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Title: DynamicBHR3 FLAG Implementation

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DynamicBHR3 FLAG Implementation

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- Thanks to Juan Saenz (XCP-4) for running the xRAGE simulations used in these comparisons
- Thanks to Nick Denissen (XTD-PRI) for technical input regarding FLAG turbulence modeling

Outline

- Taylor Green Vortex (TGV) test problem
- ILES FLAG/xRAGE comparisons
- DynamicBHR3 FLAG/xRAGE comparisons
- FLAG BHR3 and DynamicBHR3 resolution studies
- Conclusions
- Future Work

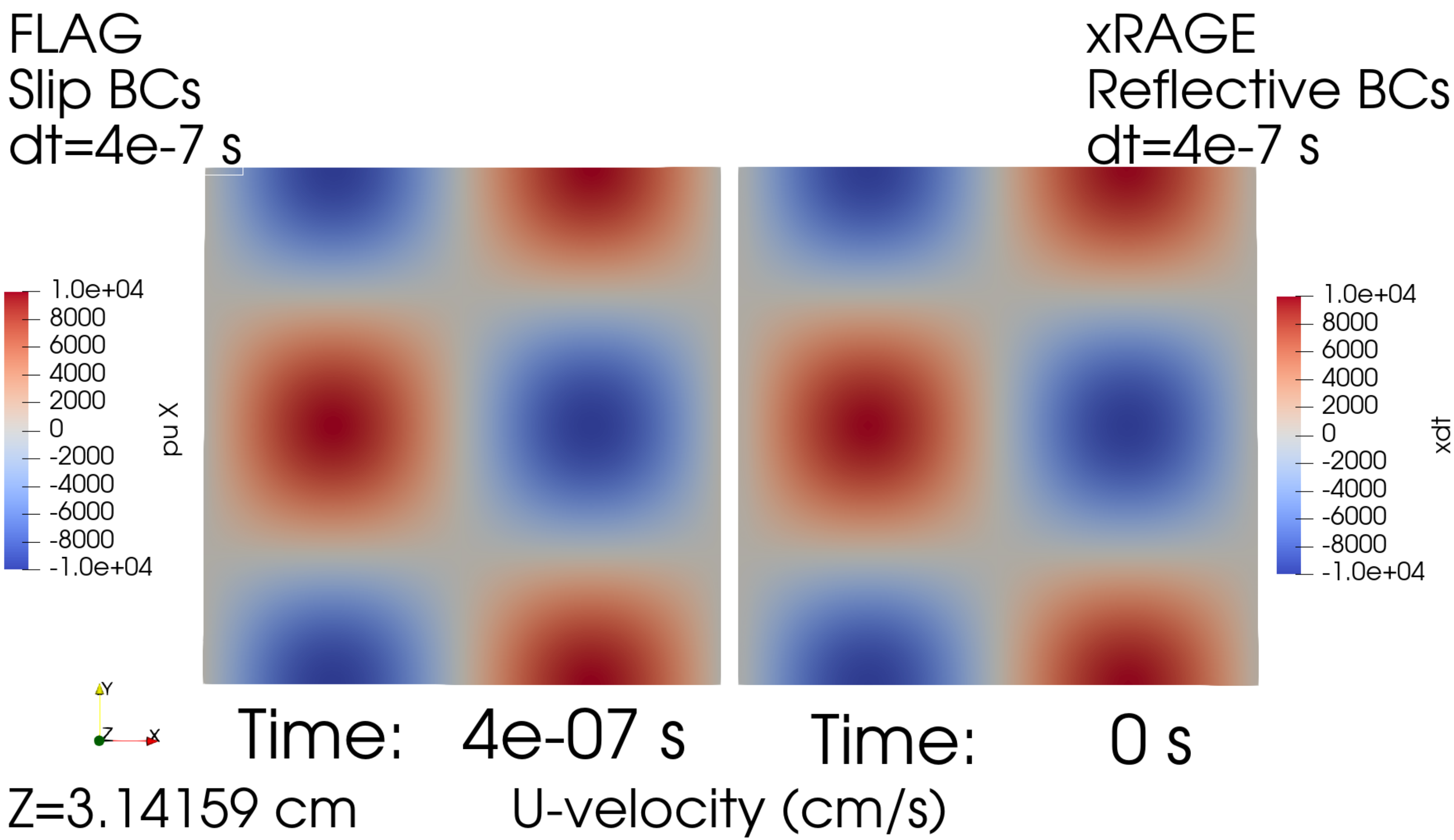
Taylor Green Vortex Test Problem

- The flow develops, transitions to turbulent, and then dissipates; peak turbulent dissipation at ~ 1 ms, total of 3 ms simulation time
- 3D Cartesian mesh: baseline 64^3 resolution over a (2*pi)^3 sized domain
- FLAG uses slip BCs (normal component fixed, tangential component free) and xRAGE uses periodic BC; similar approaches
- Solving the Euler equations (no physical viscosity), so there are **different effective Reynolds numbers** between the codes based on their respective numerical dissipation
- FLAG operates in pure Eulerian mode (remaps to the original mesh location)
- Gamma-law gas with gamma = 1.4

ILES FLAG/xRAGE Comparisons

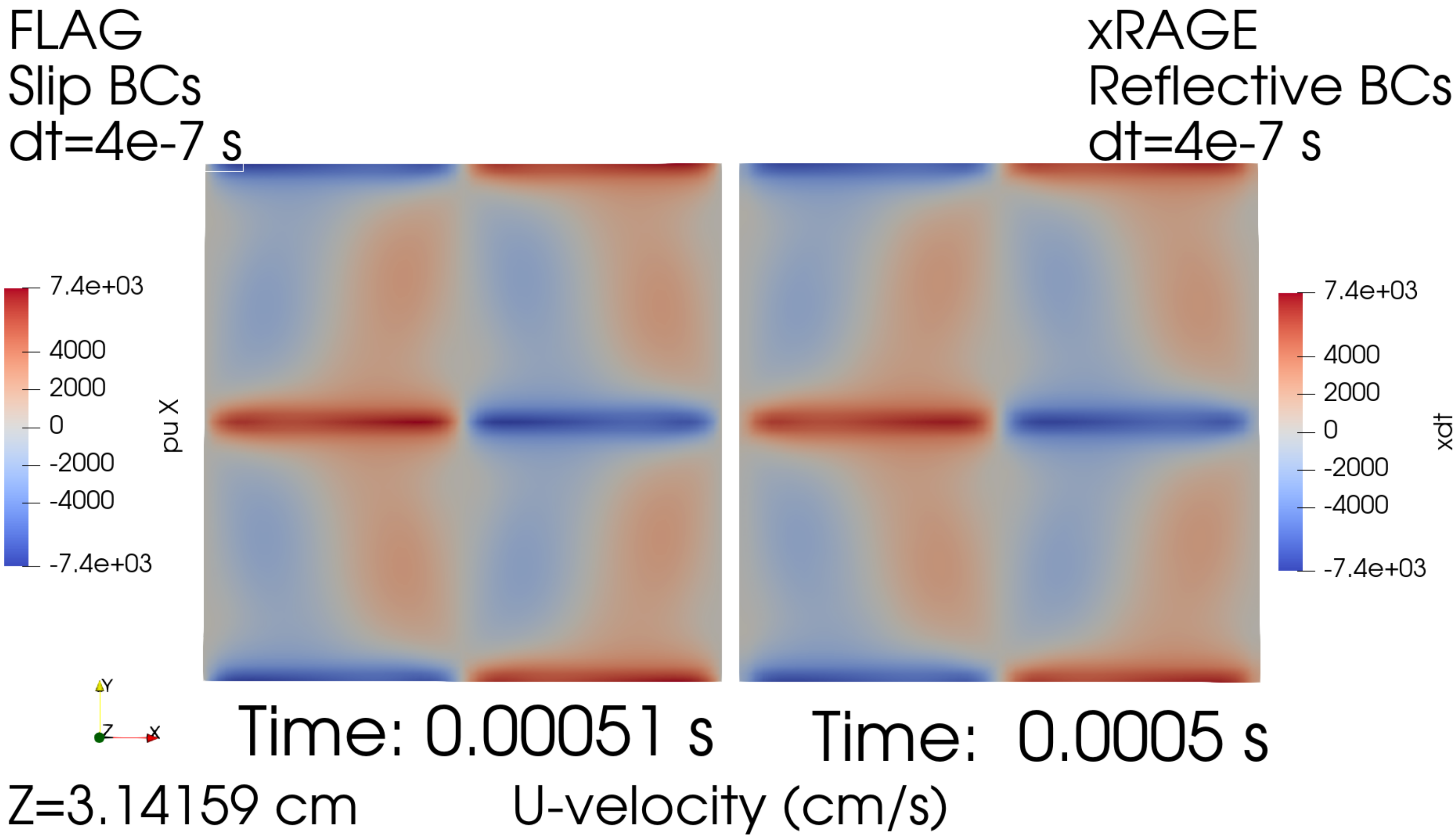
- No turbulence models – Implicit Large Eddy Simulation (ILES)
- Comparing baseline hydrodynamics of the codes on a flow that transitions to turbulent
- xRAGE has periodic BCs while FLAG has slip BCs (similar for this case)
- Time step held constant at 4e-7 s to avoid differences due to temporal discretization
- This next sequence of comparisons between FLAG/xRAGE demonstrate the differences observed in the codes due to different effective Reynolds numbers (no physical viscosity so the numerical dissipation acts as the only dissipation, effectively setting the respective Reynolds number)

U-velocity Component, Z center plane

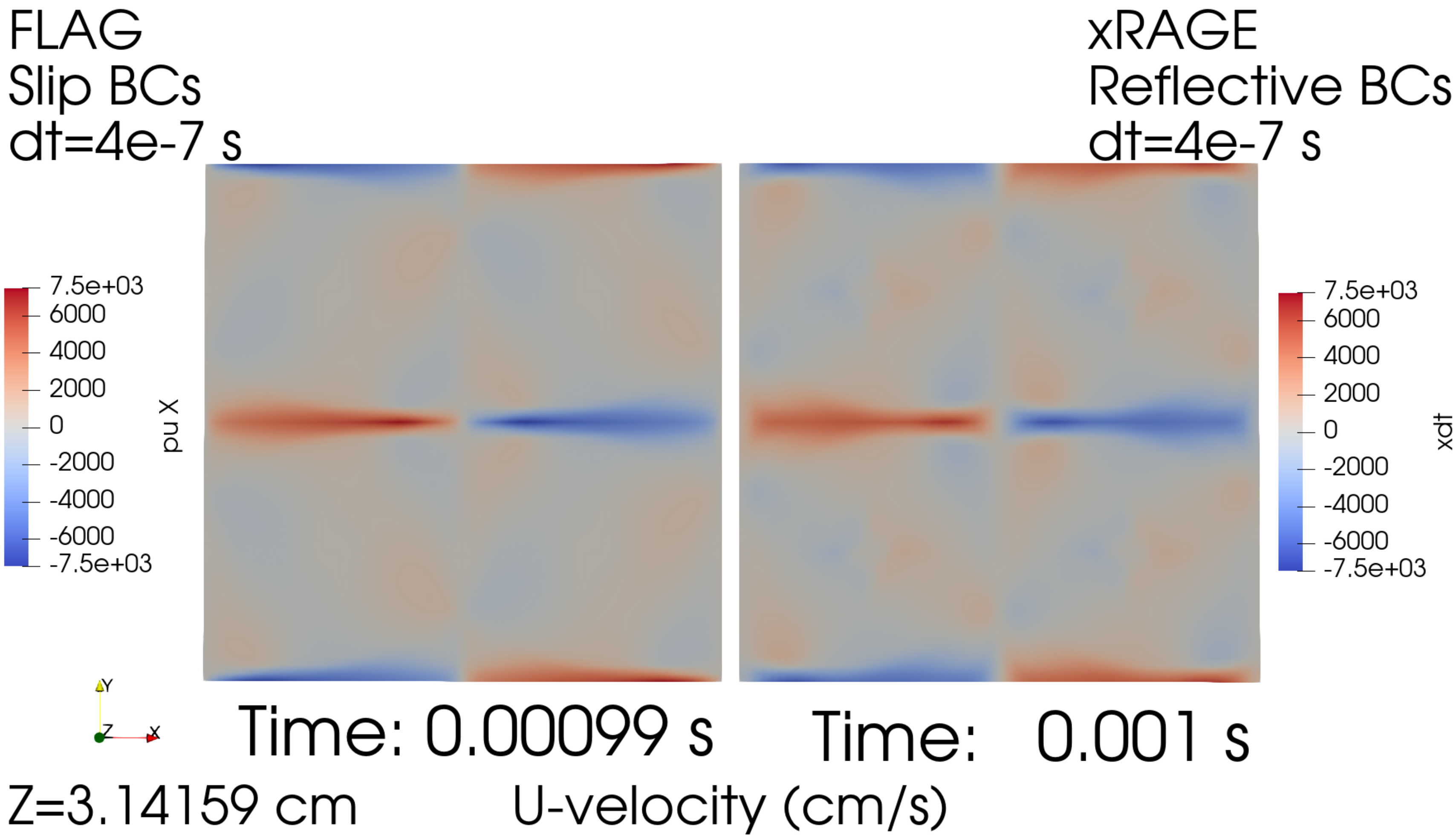


FLAG output is one time step ahead; essentially the same

U-velocity Component, Z center plane



U-velocity Component, Z center plane



Good qualitative agreement up to this point (transitioning to turbulent)

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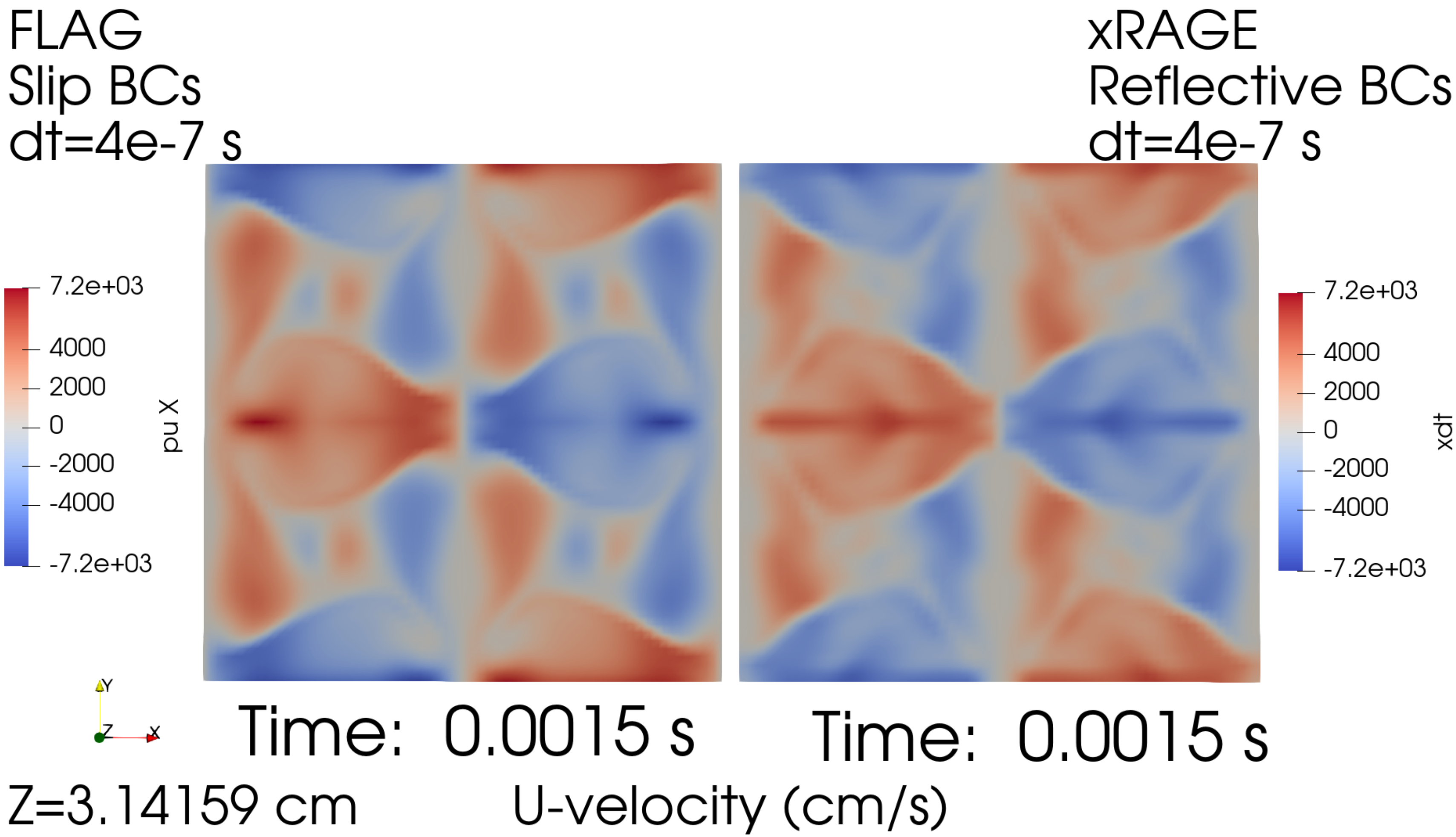
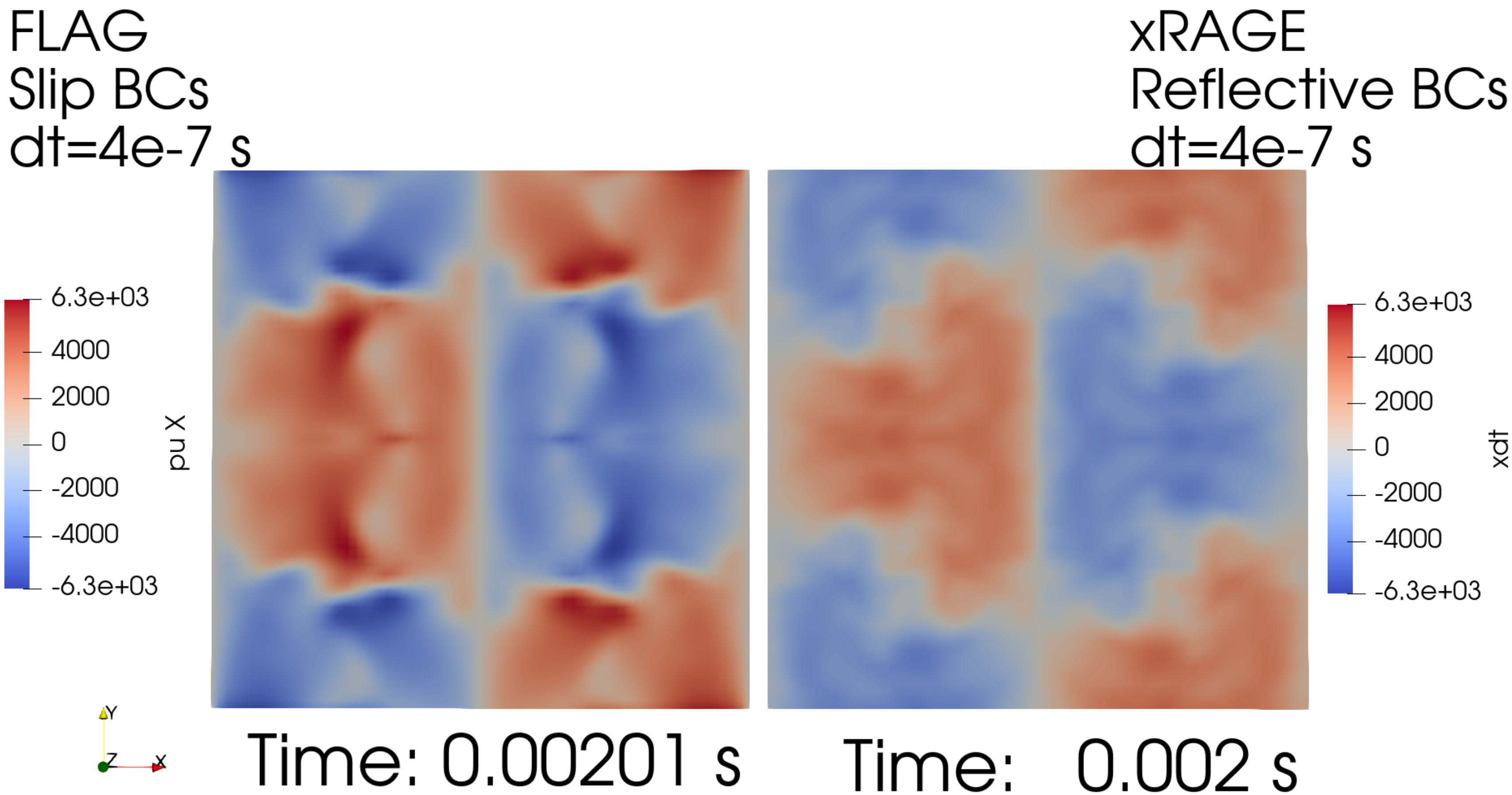
U-velocity Component, Z center plane



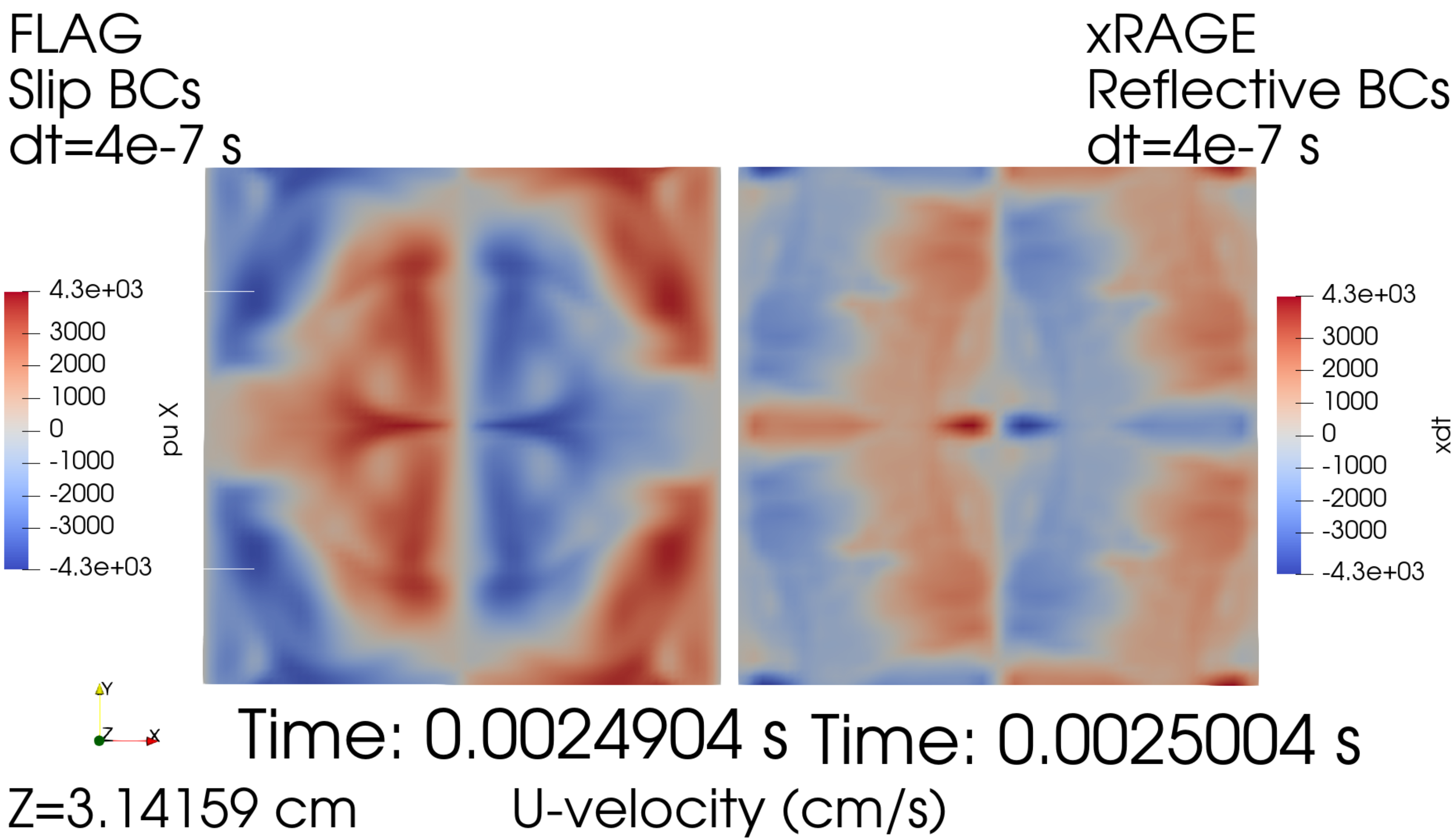
Starting to see some qualitative differences

U-velocity Component, Z center plane

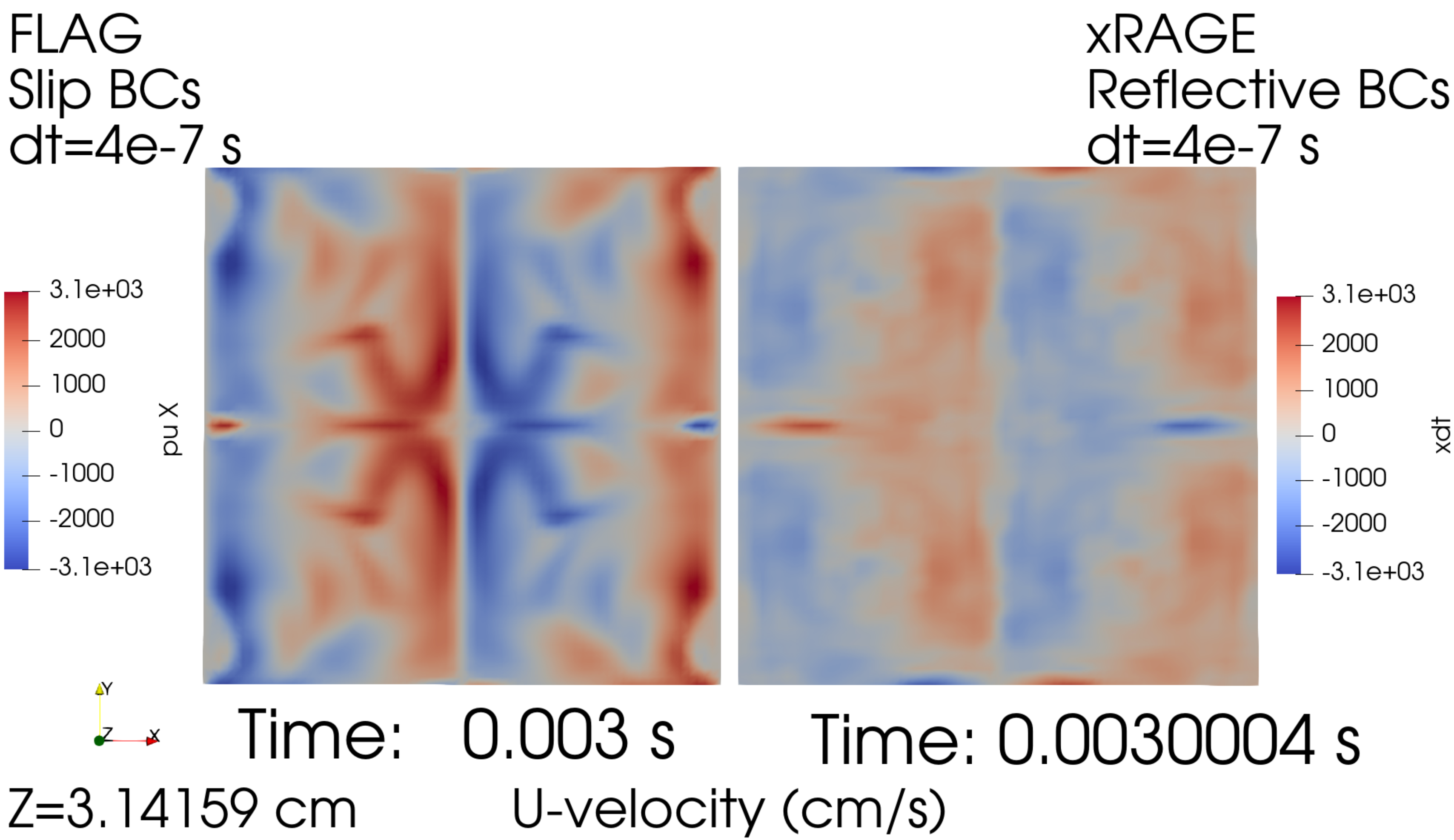


Z=3.14159 cm U-velocity (cm/s)

U-velocity Component, Z center plane



U-velocity Component, Z center plane

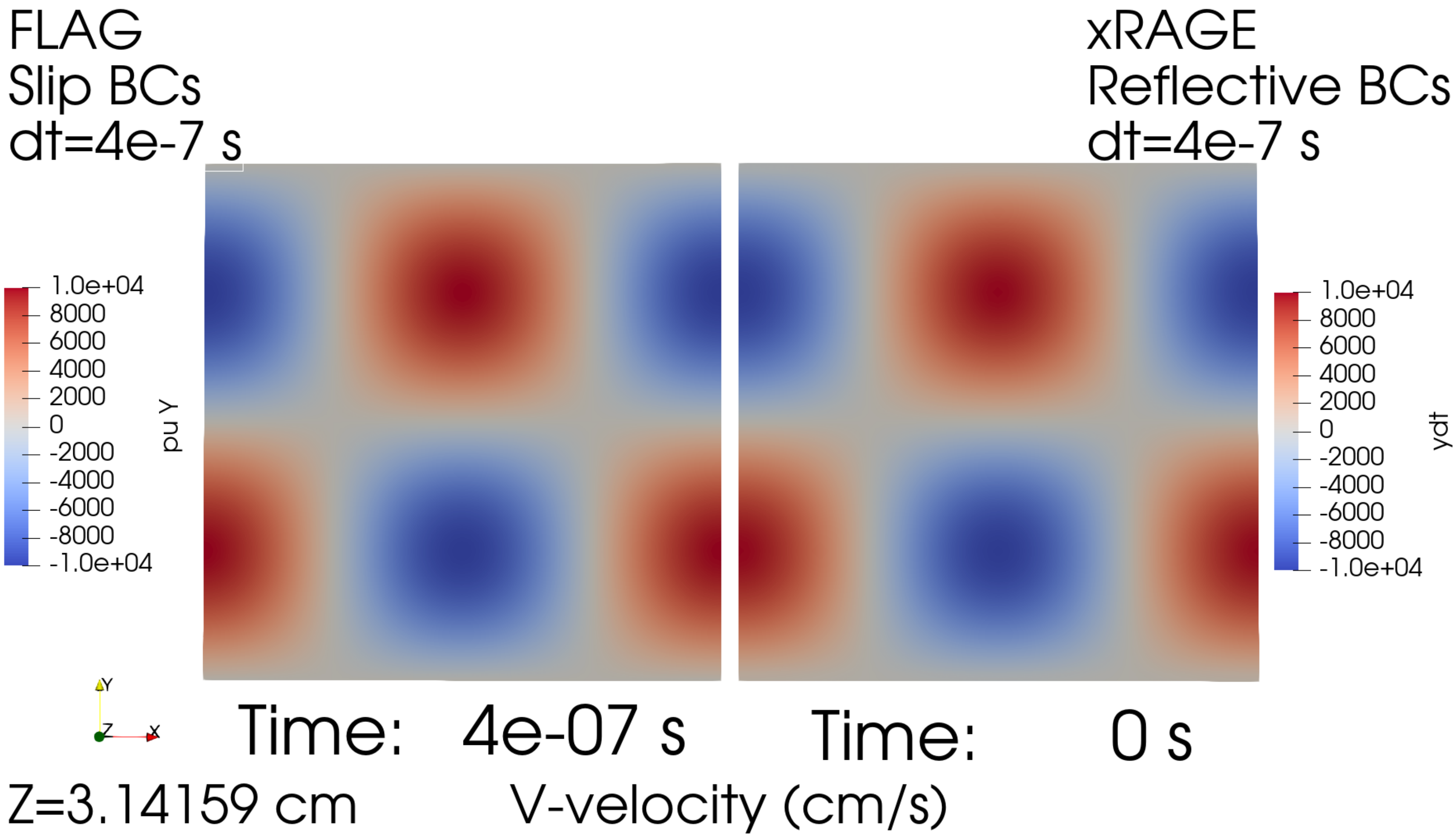


Results are quite different this late in time

U-velocity Component, Z center plane

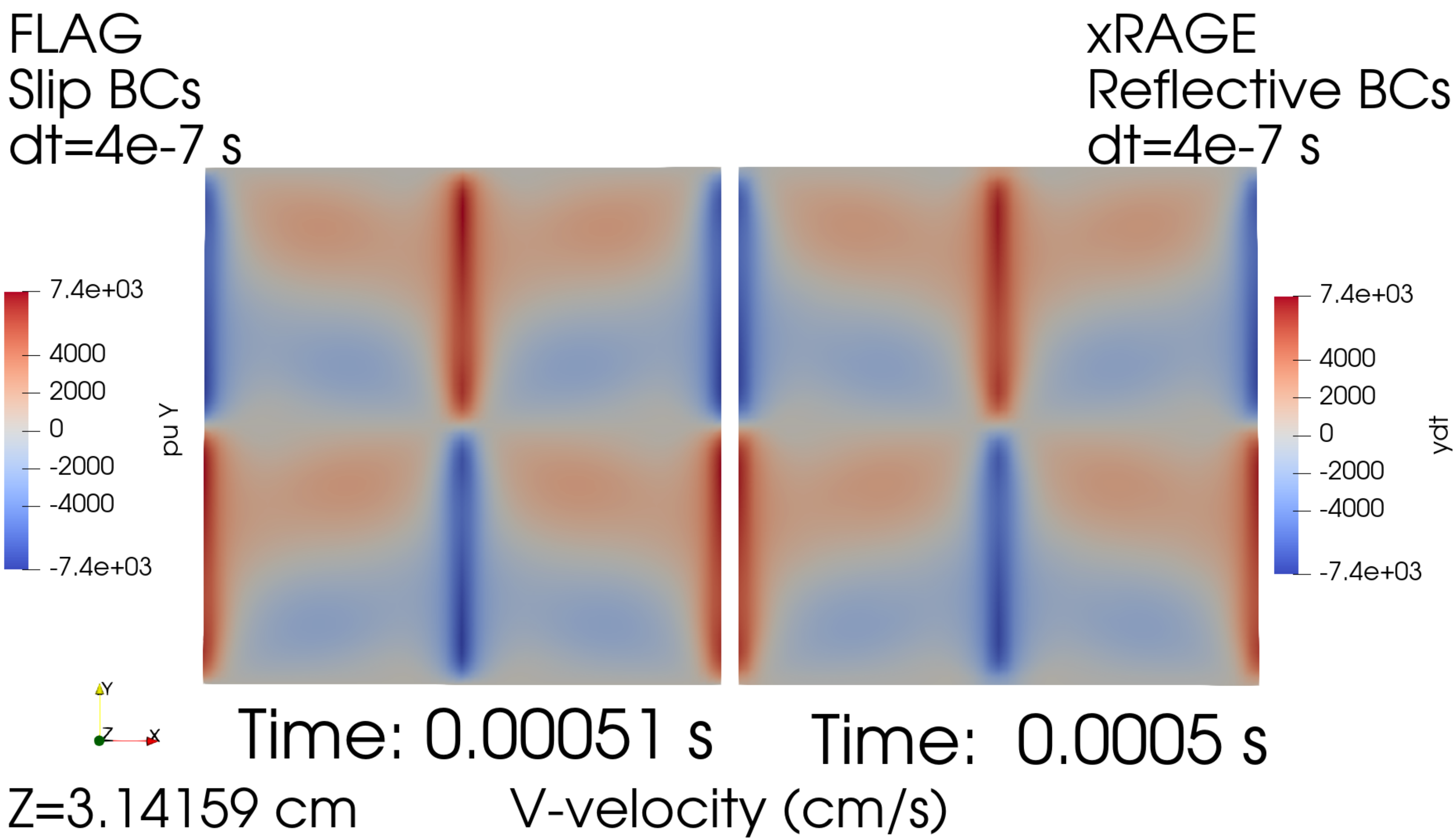
- Good qualitative agreement up to ~1 ms, after which differences become more pronounced as the flow becomes turbulent
- KE peak dissipation occurs at ~1 ms
- Initialization is consistent between codes
- Minor differences in BCs between codes are negligible

V-velocity Component, Z center plane

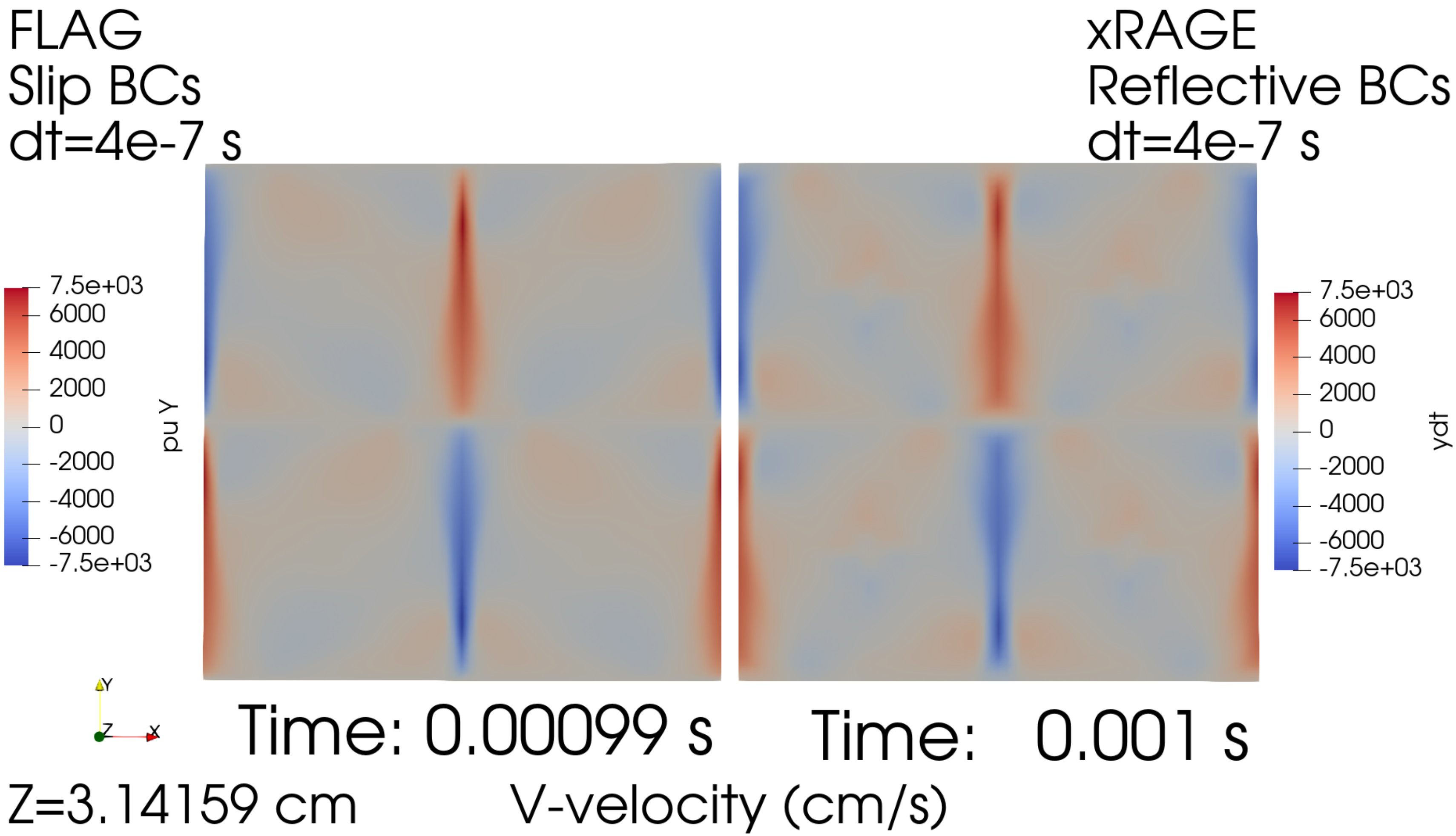


FLAG output is one time step ahead; essentially the same

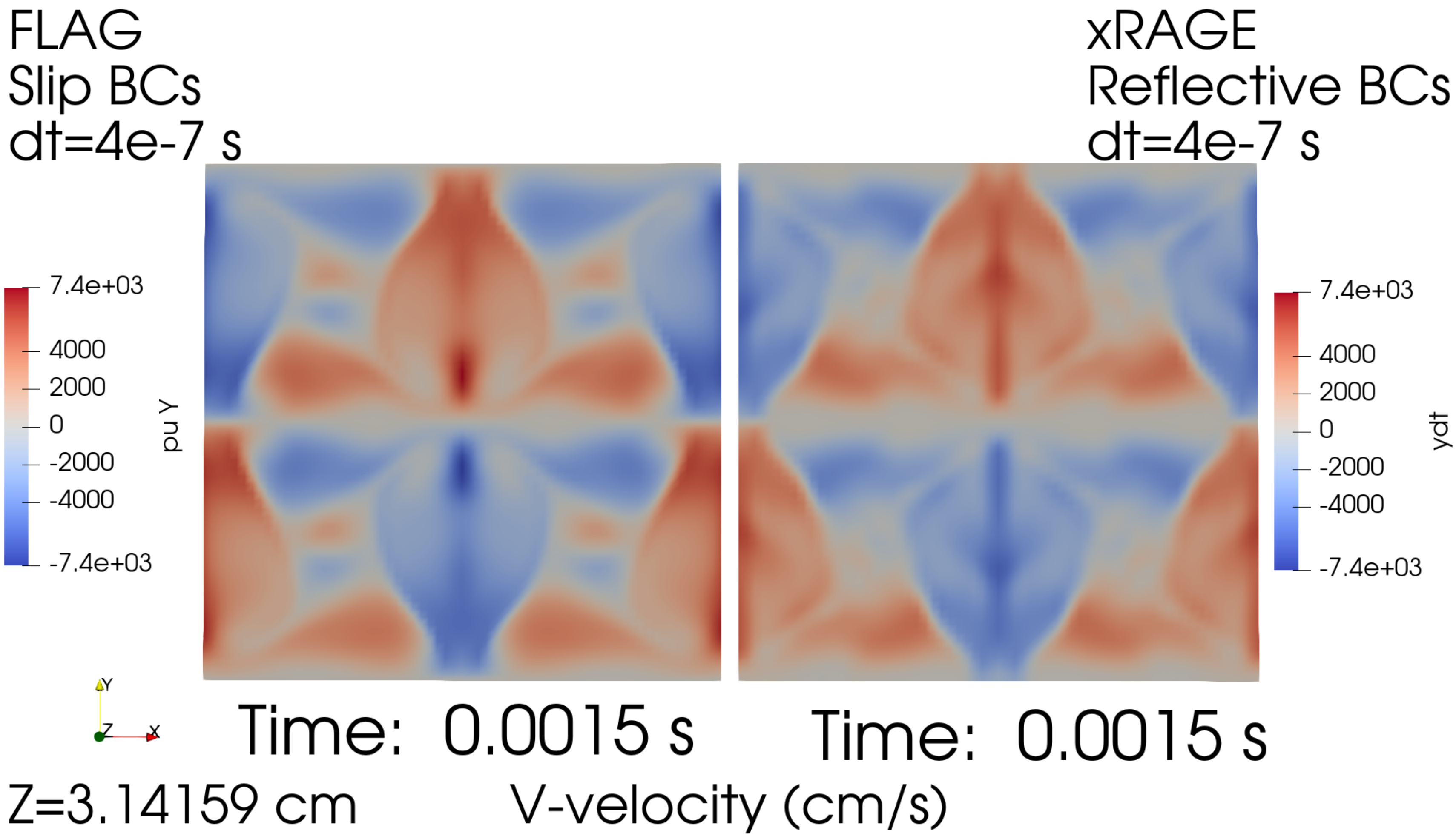
V-velocity Component, Z center plane



V-velocity Component, Z center plane

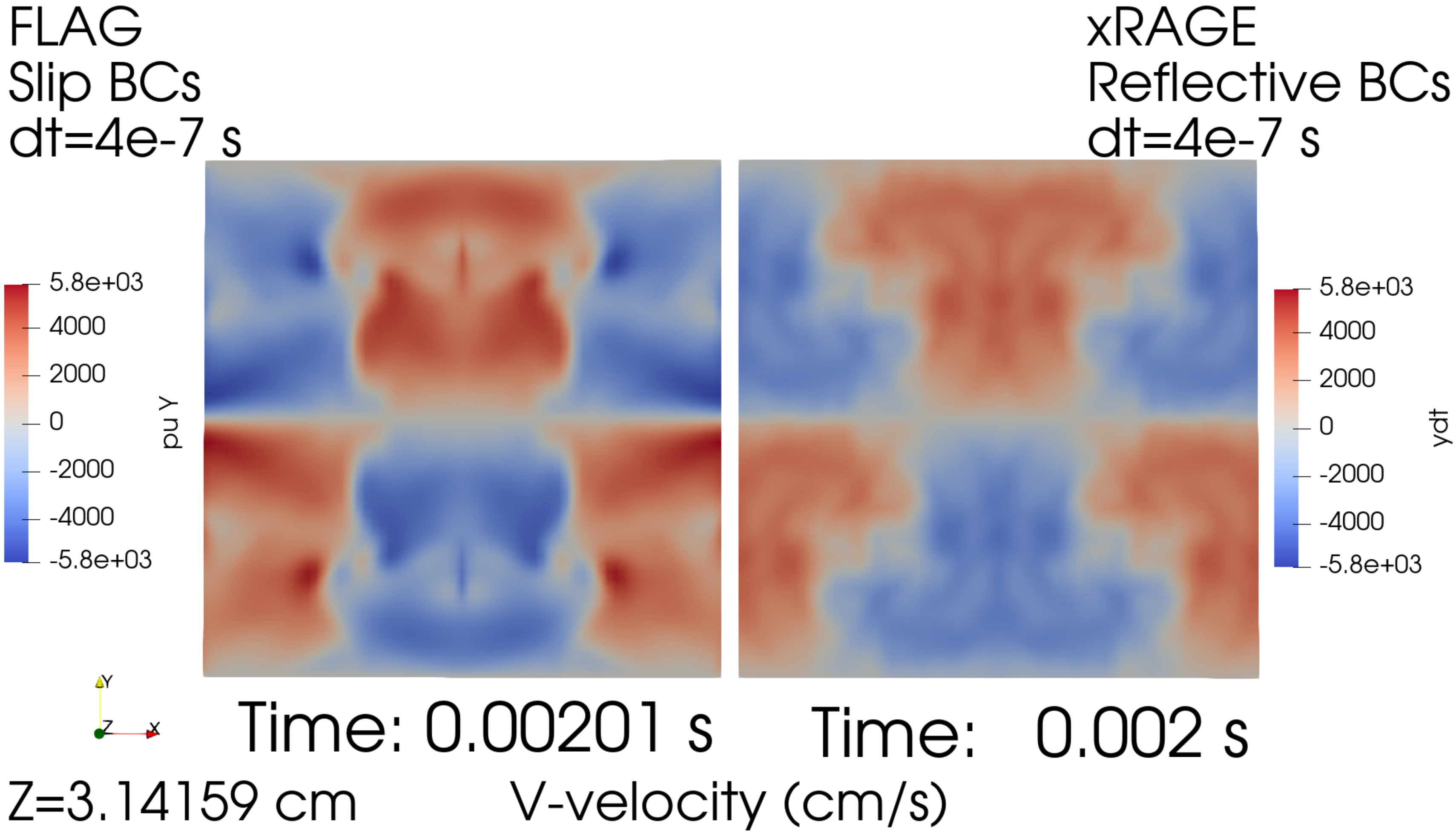


V-velocity Component, Z center plane

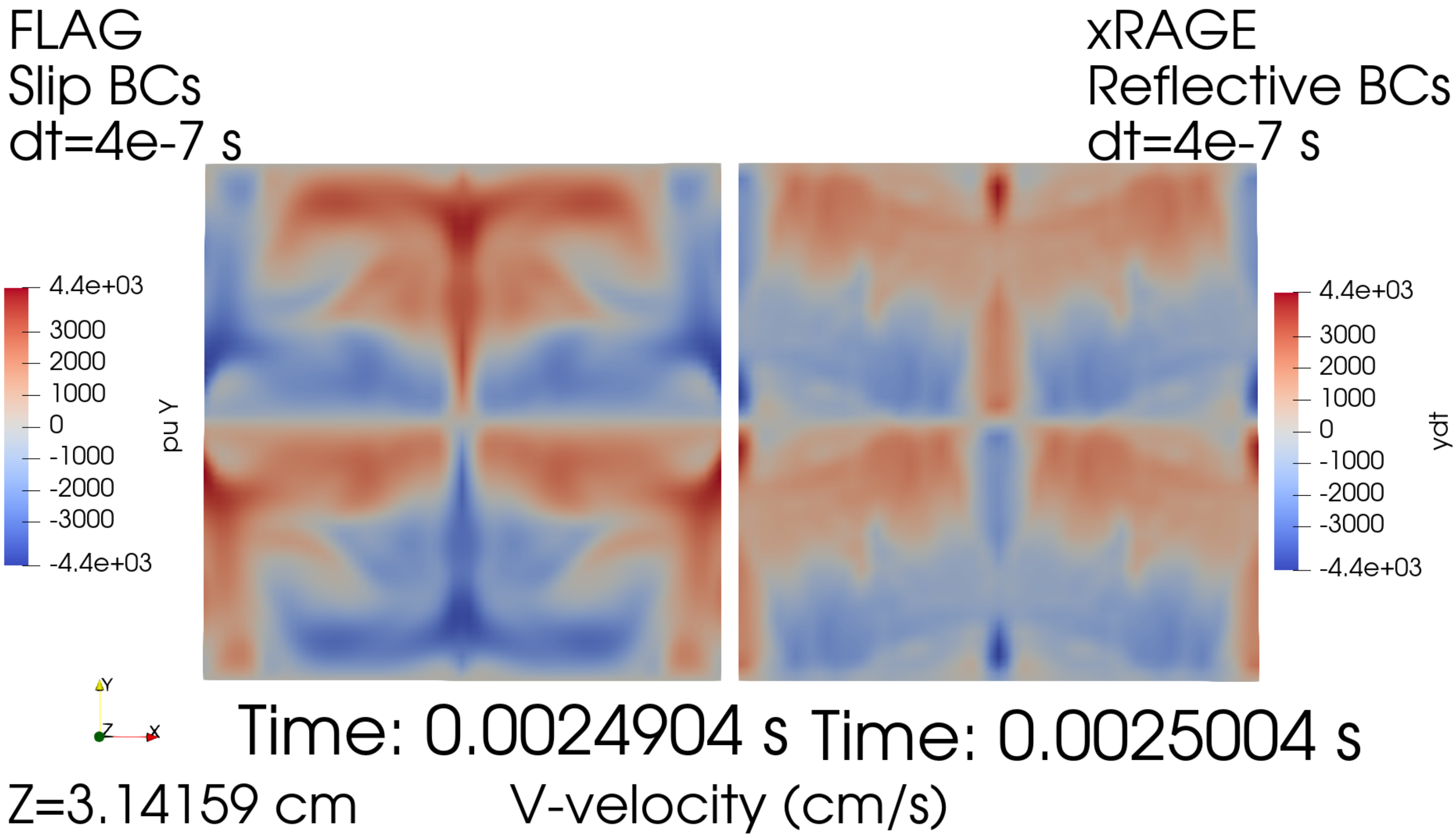


Qualitative differences are starting to appear at this point

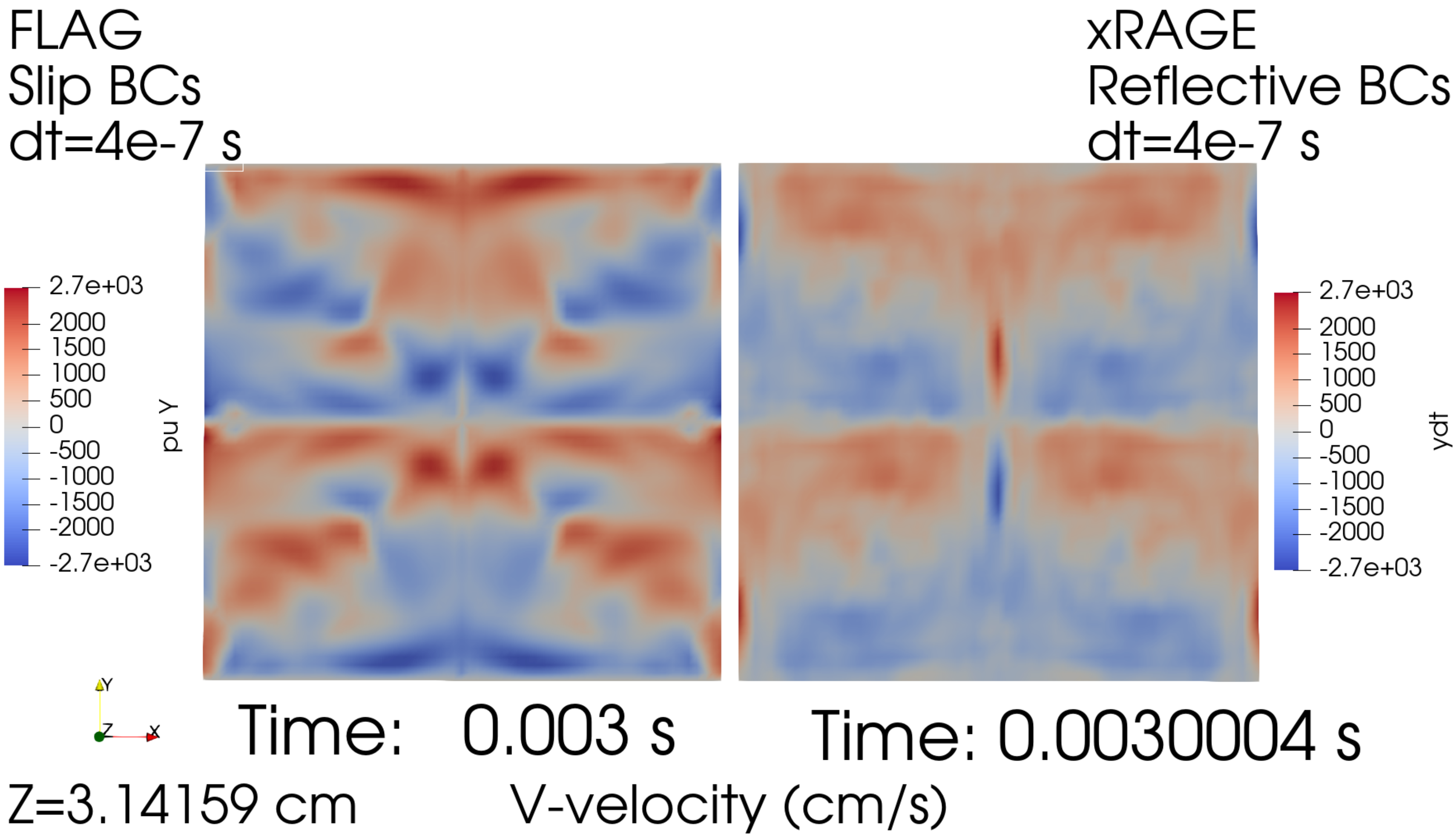
V-velocity Component, Z center plane



V-velocity Component, Z center plane



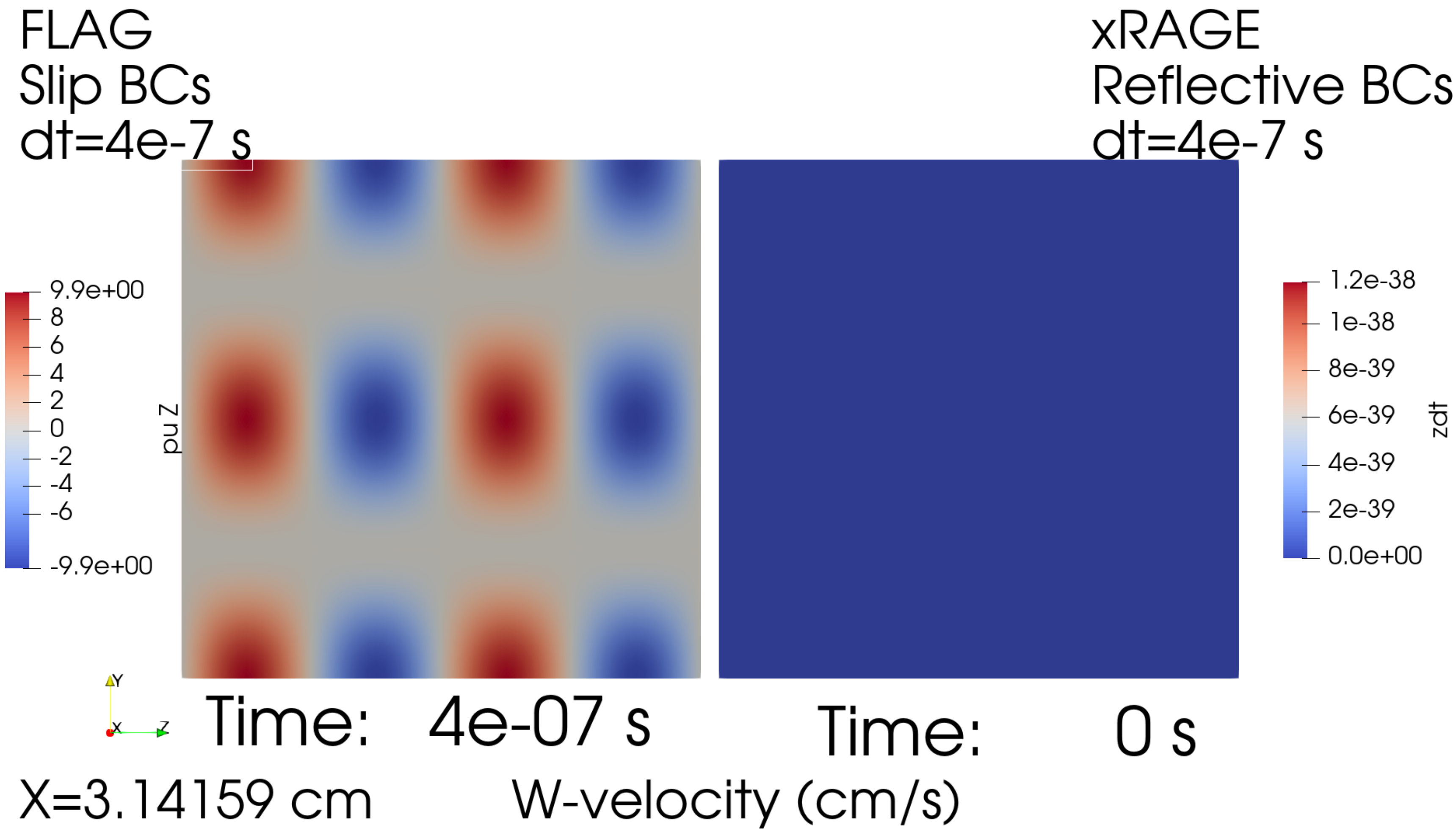
V-velocity Component, Z center plane



V-velocity Component, Z center plane

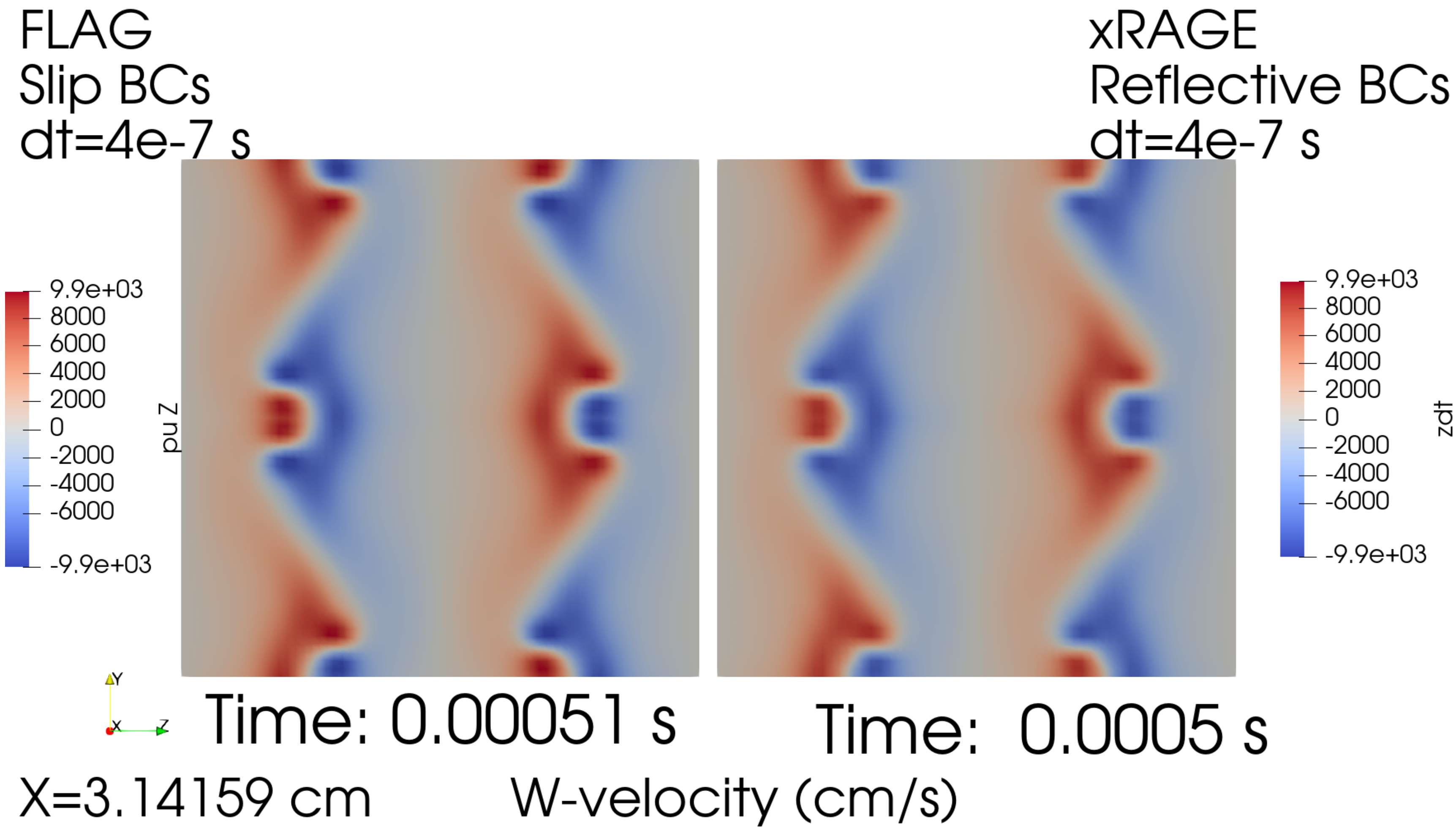
- Similar observations as U-velocity component
- Good qualitative agreement up to ~1 ms, after which differences become more pronounced after the flow becomes turbulent
- KE peak dissipation occurs at ~1 ms
- Initialization is consistent between codes
- Minor differences in BCs between codes are negligible

W-velocity Component, X center plane

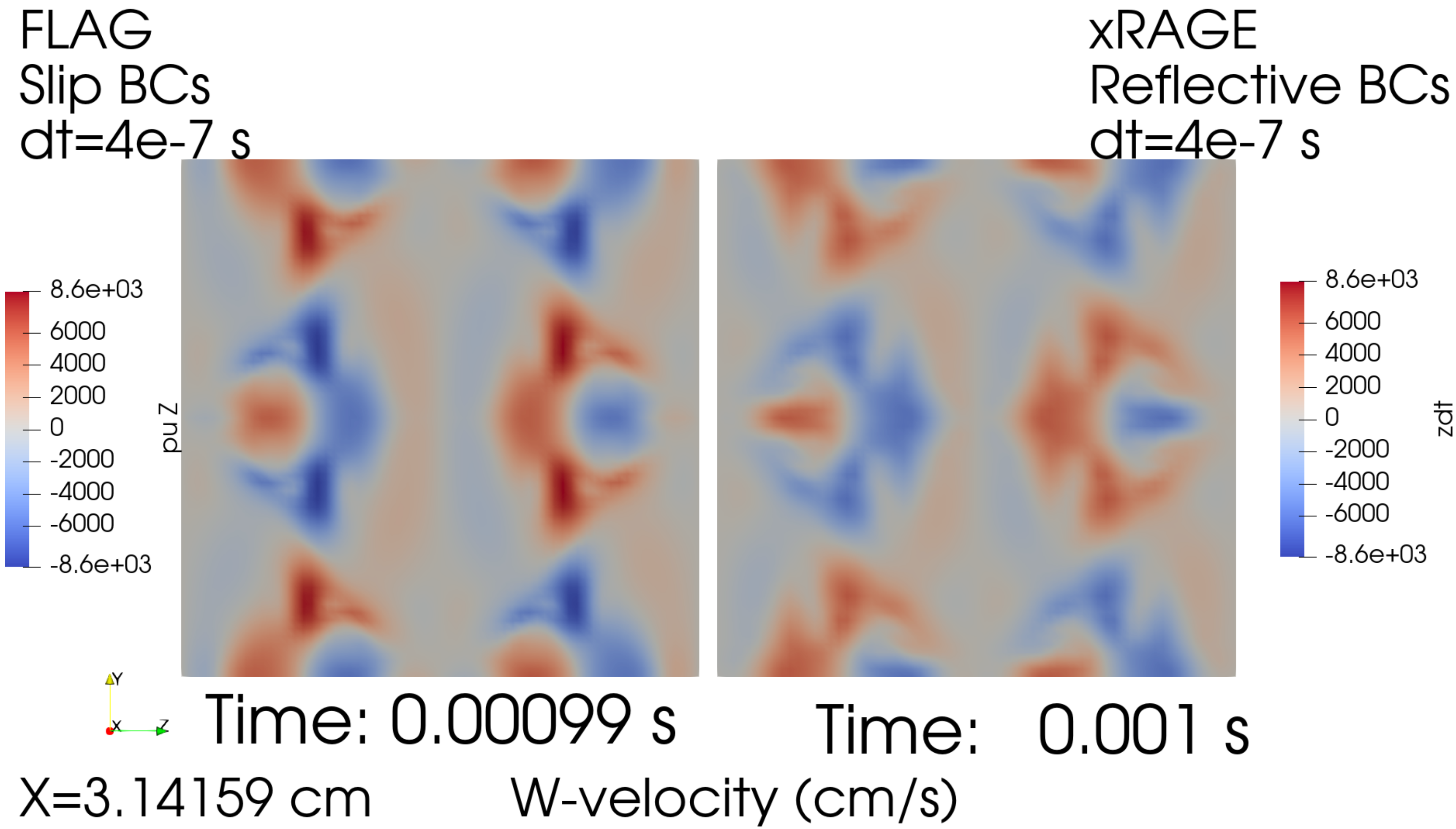


*FLAG output is after one time step, so w-velocity has started to develop (it's initialized to 0).

W-velocity Component, X center plane



W-velocity Component, X center plane



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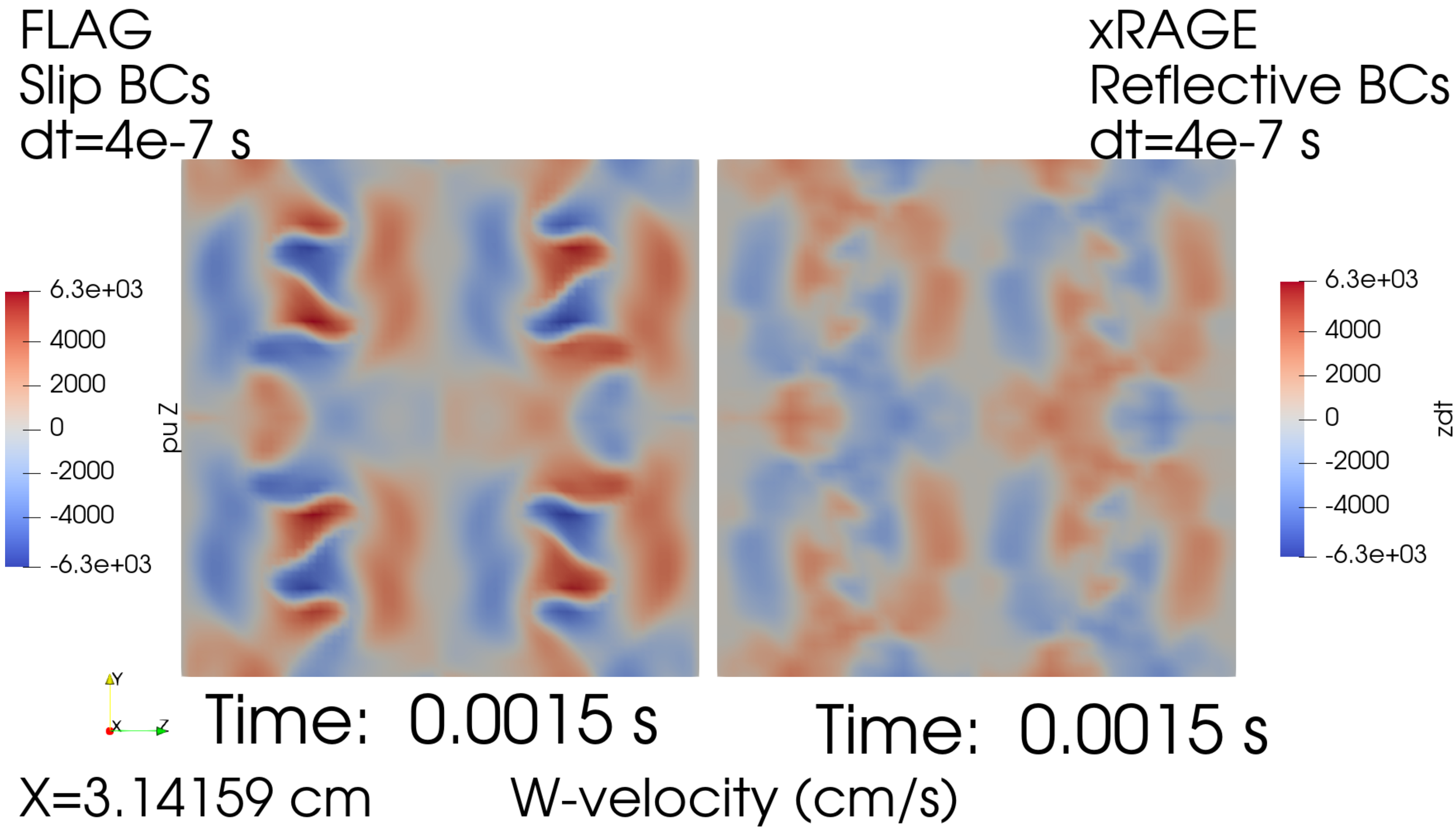
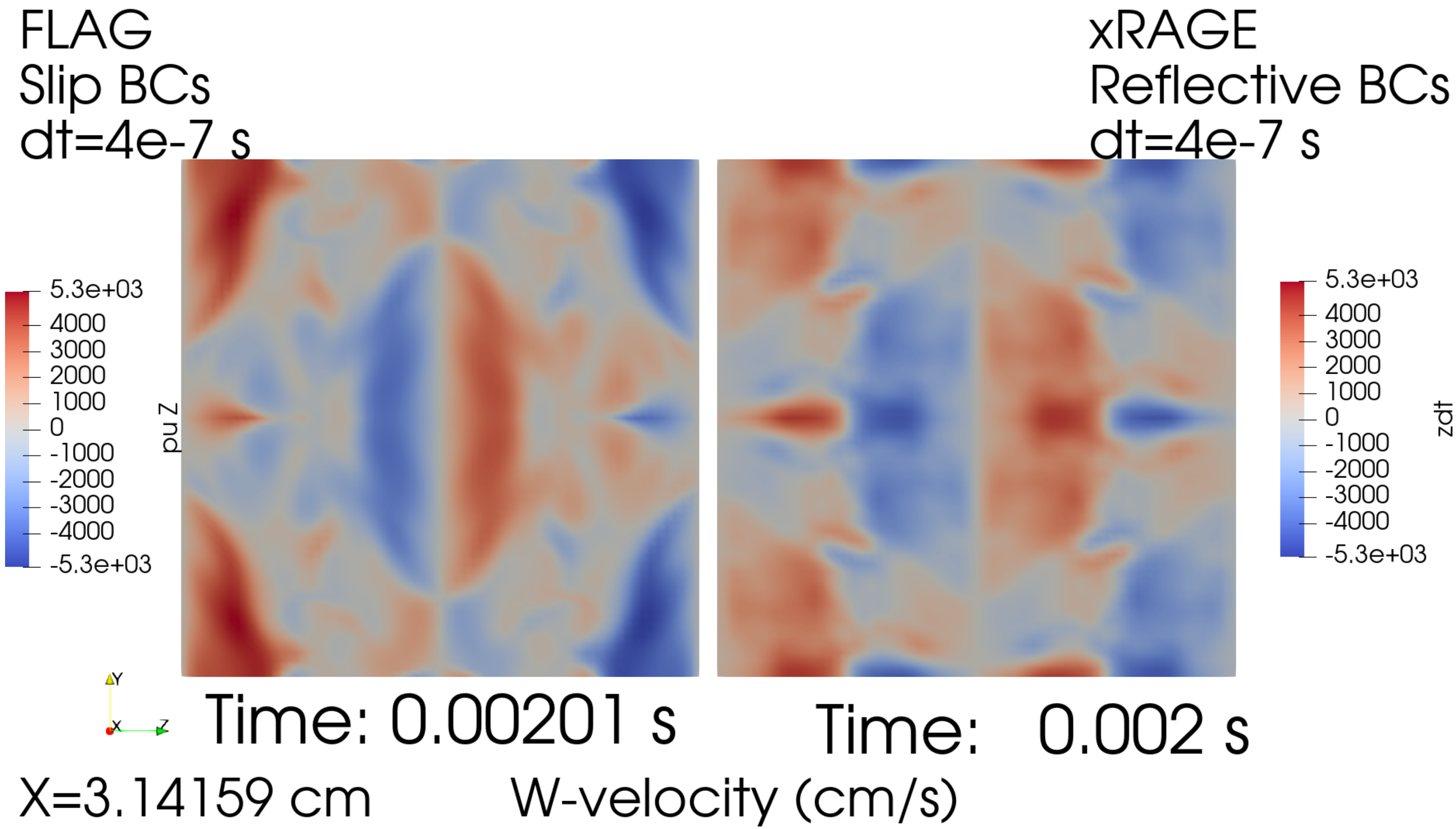
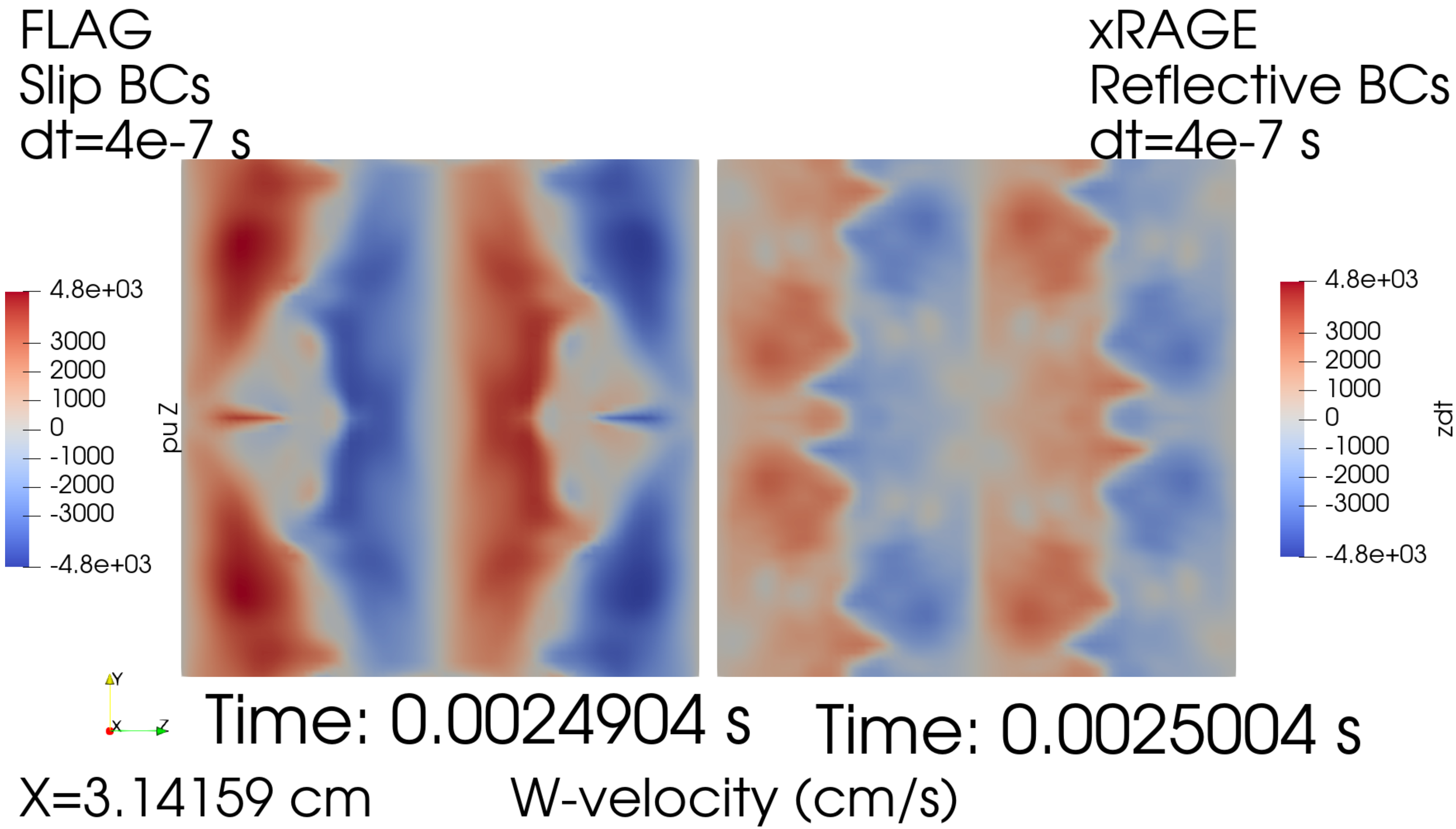
W-velocity Component, X center plane



W-velocity Component, X center plane



W-velocity Component, X center plane



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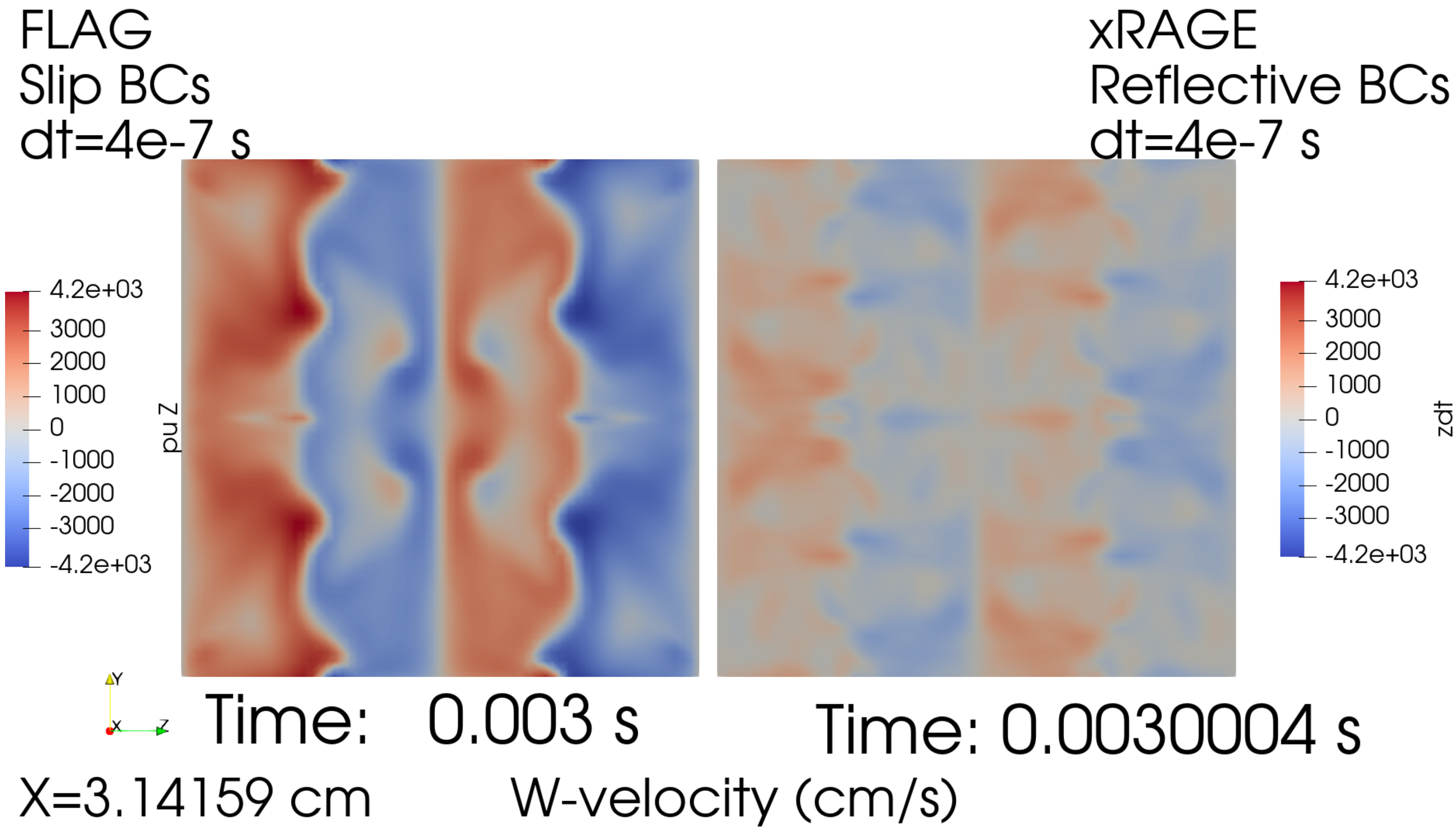
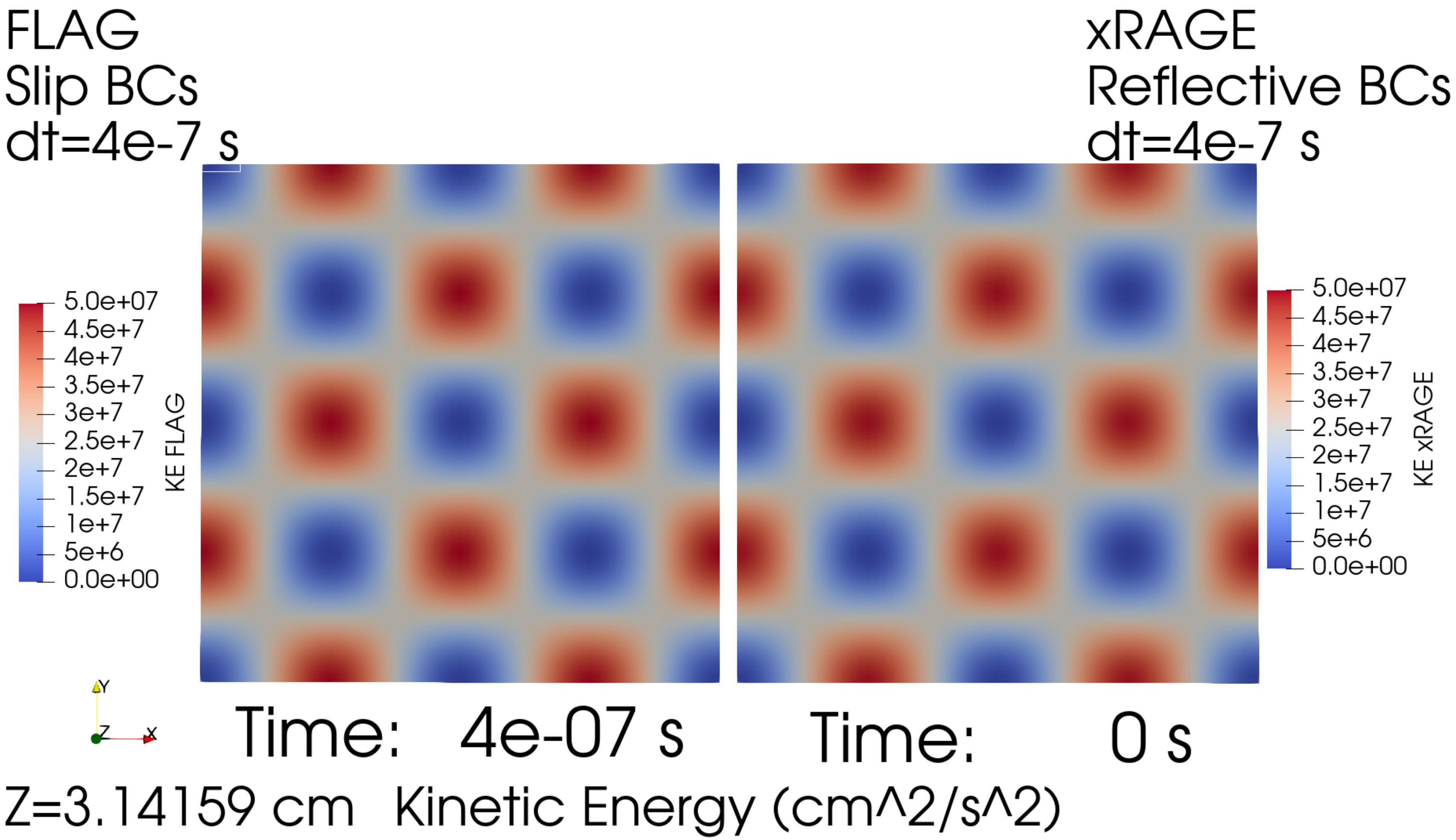
W-velocity Component, X center plane

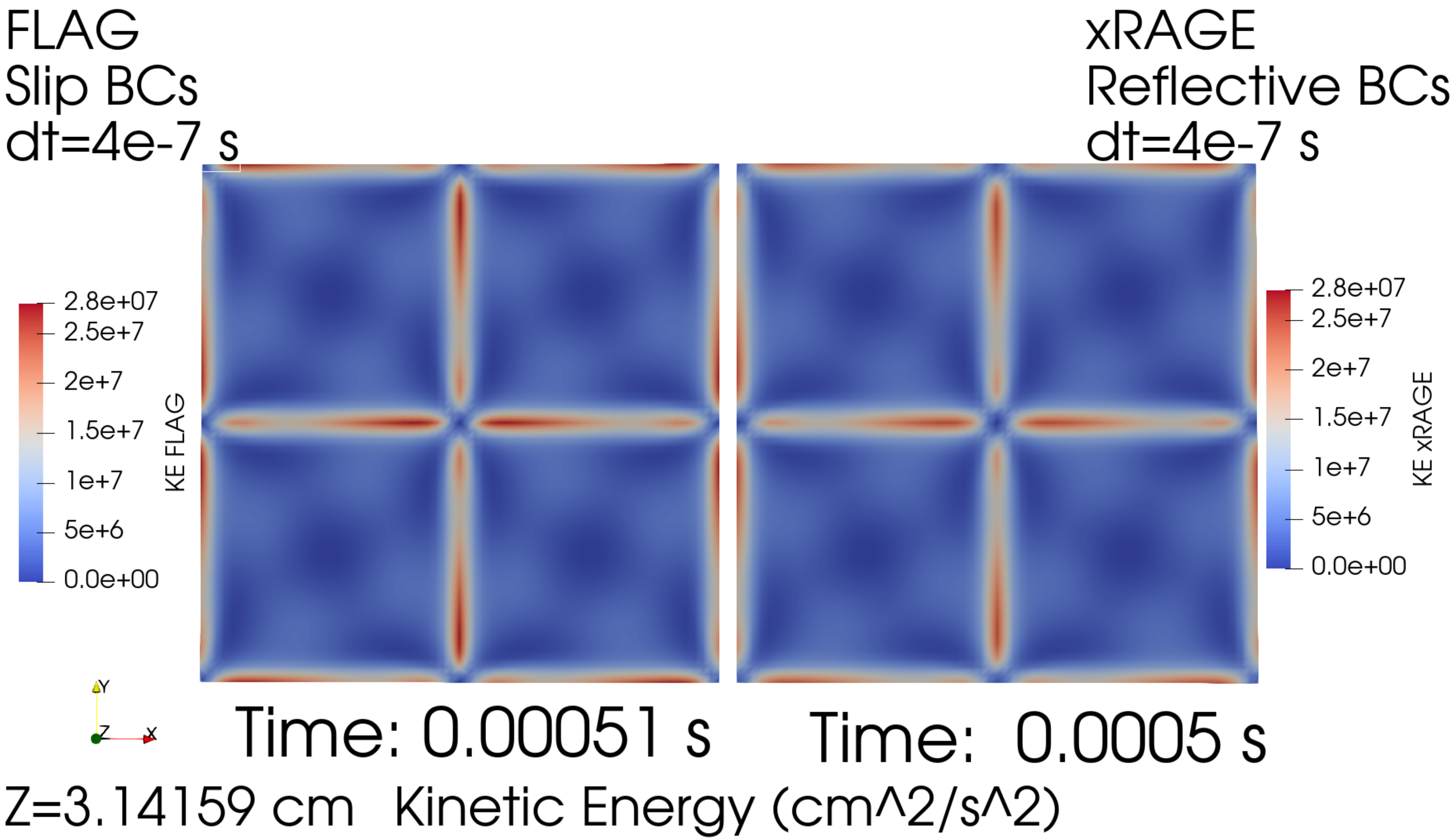


Similar observations as with the u- and v-velocity components

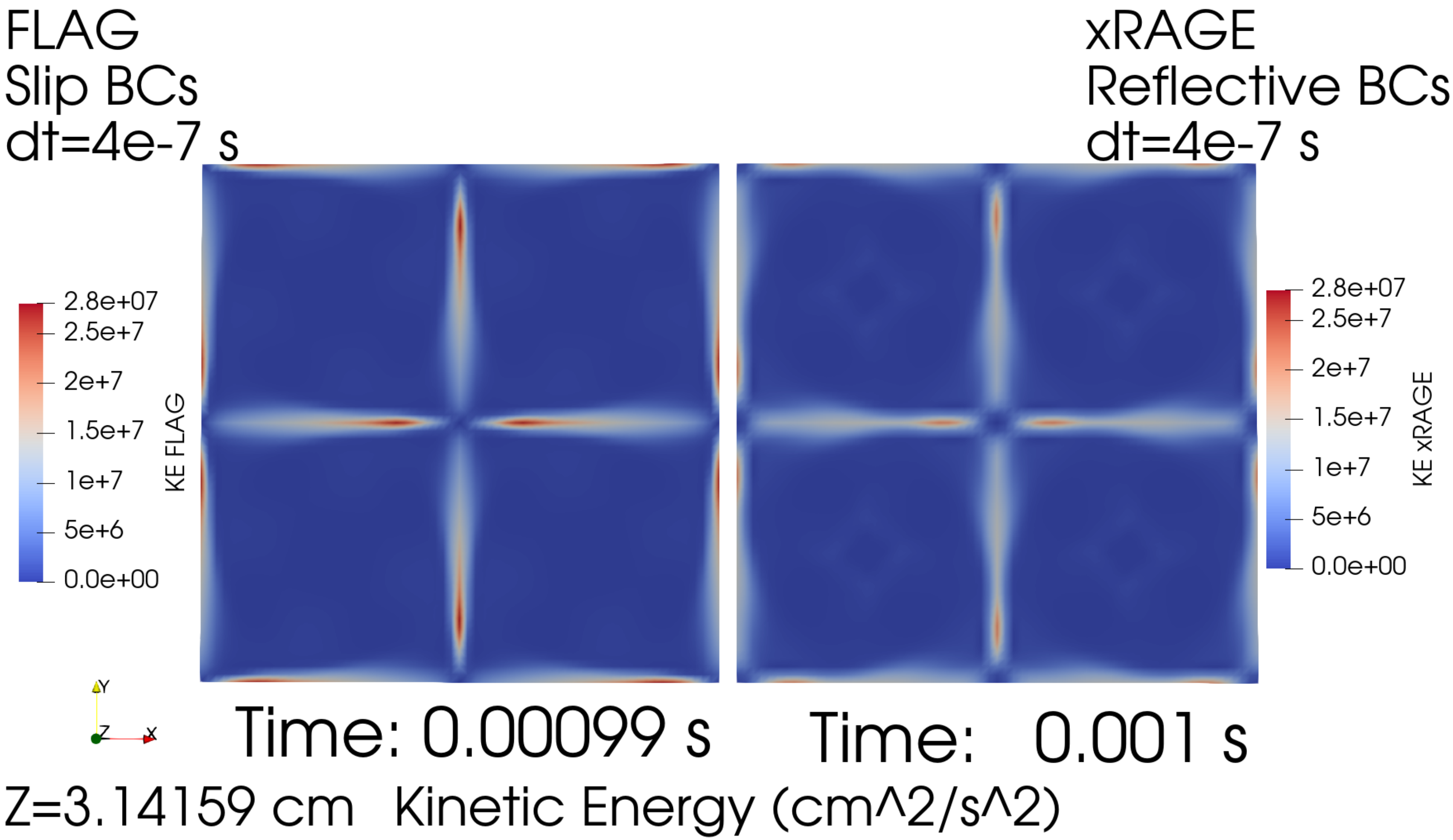
Kinetic Energy, Z center plane



Kinetic Energy, Z center plane

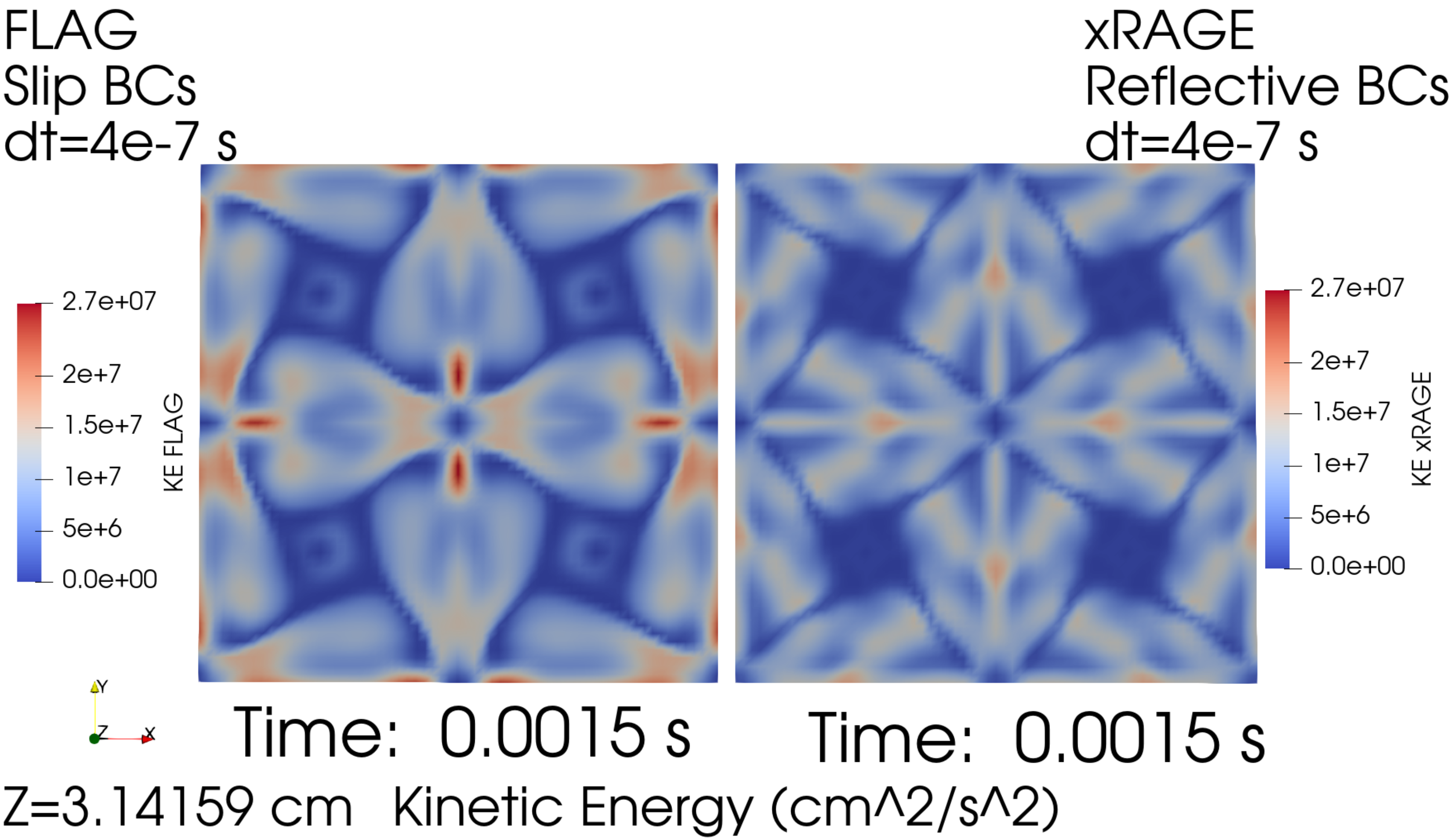


Kinetic Energy, Z center plane

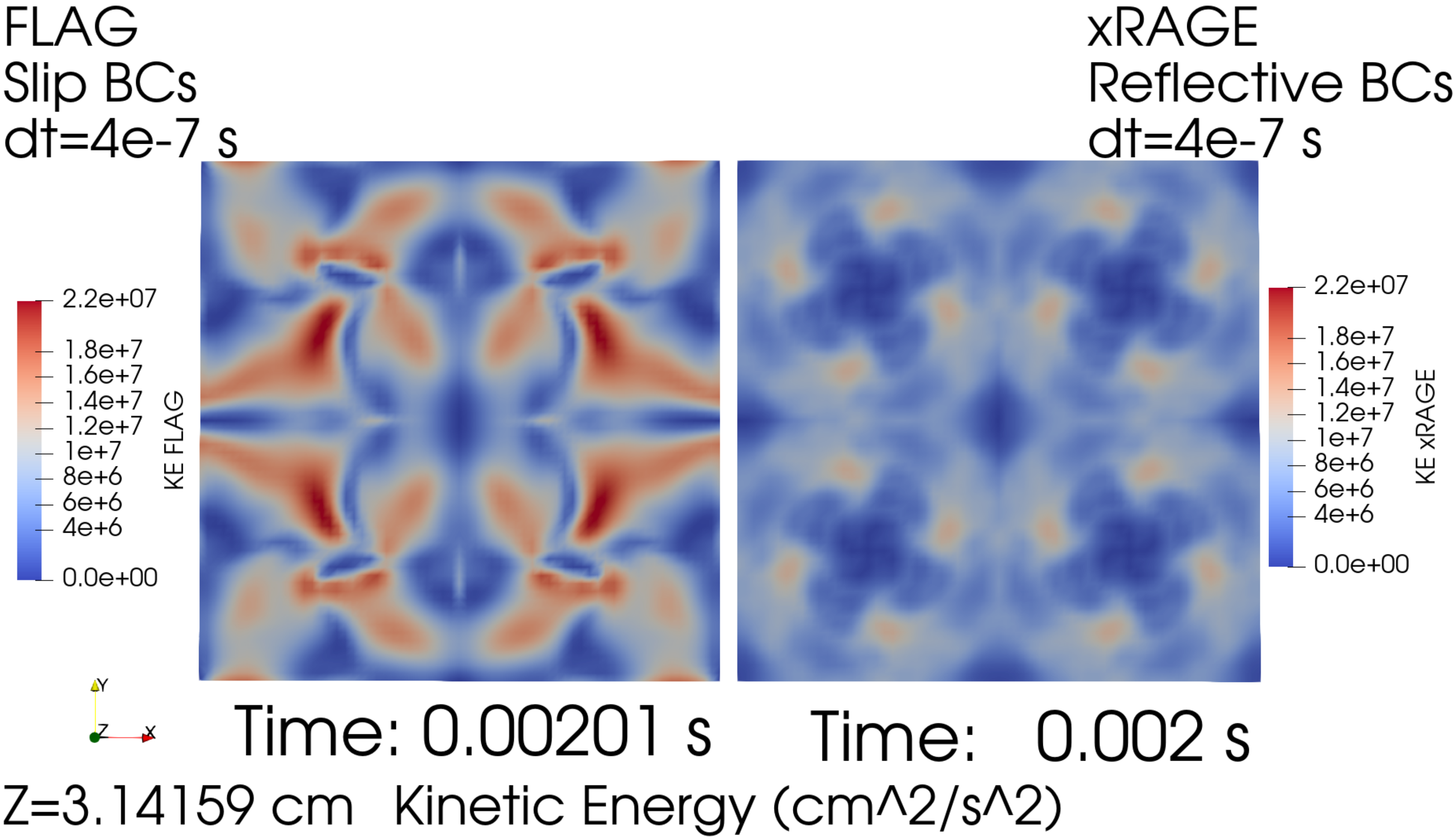


Qualitative differences noticeable at this point

Kinetic Energy, Z center plane



Kinetic Energy, Z center plane



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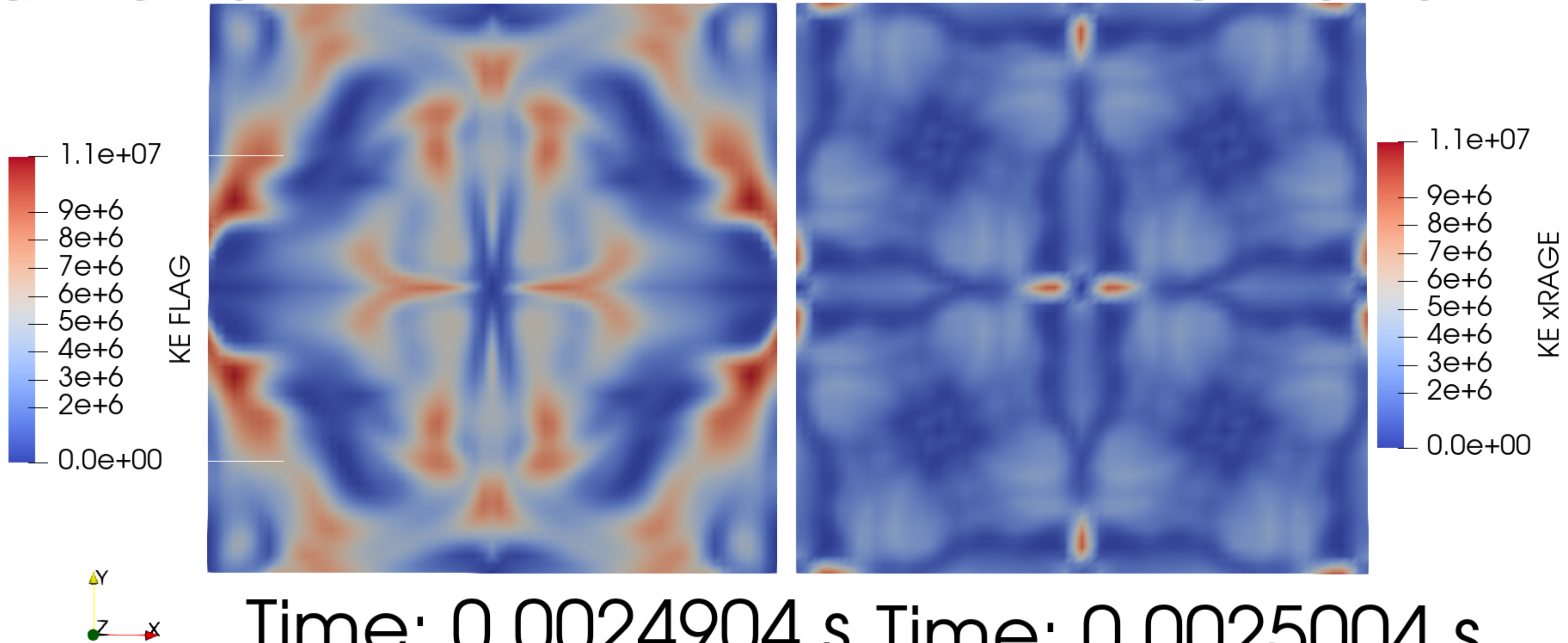
Kinetic Energy, Z center plane

FLAG
Slip BCs
dt=4e-7 s

xRAGE
Reflective BCs
dt=4e-7 s



Time: 0.0024904 s Time: 0.0025004 s

Z=3.14159 cm Kinetic Energy (cm^2/s^2)

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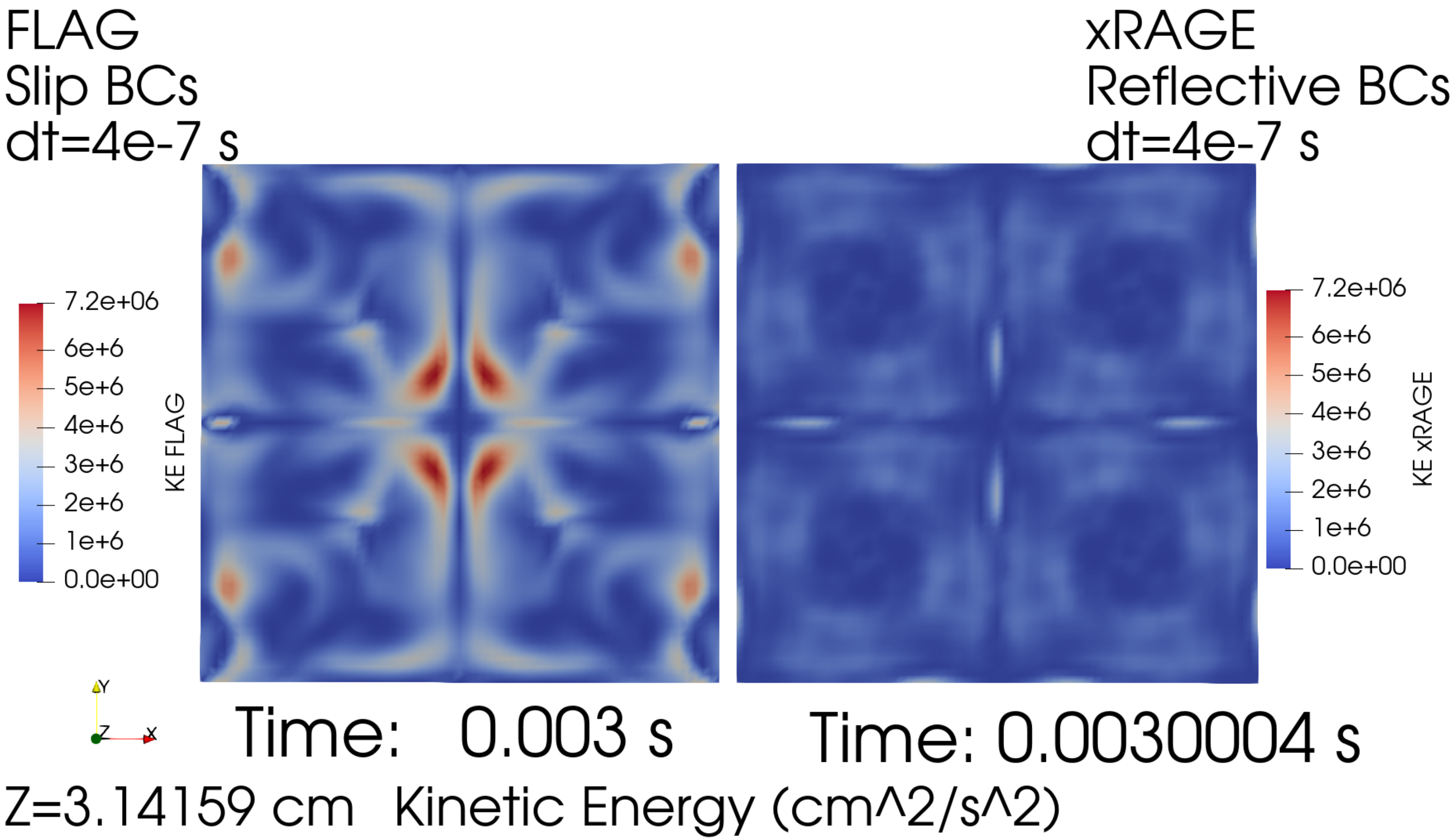
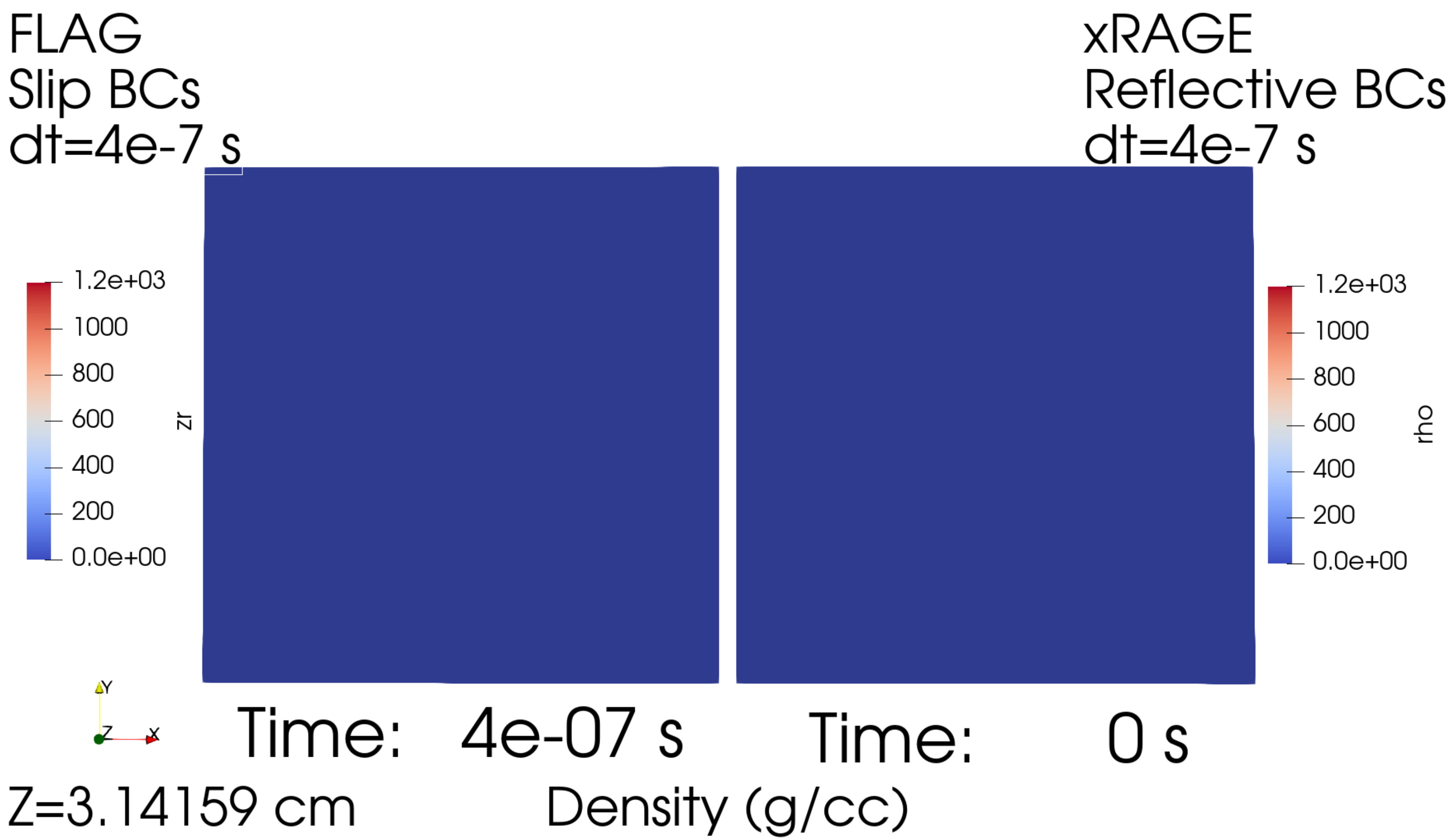
Kinetic Energy, Z center plane



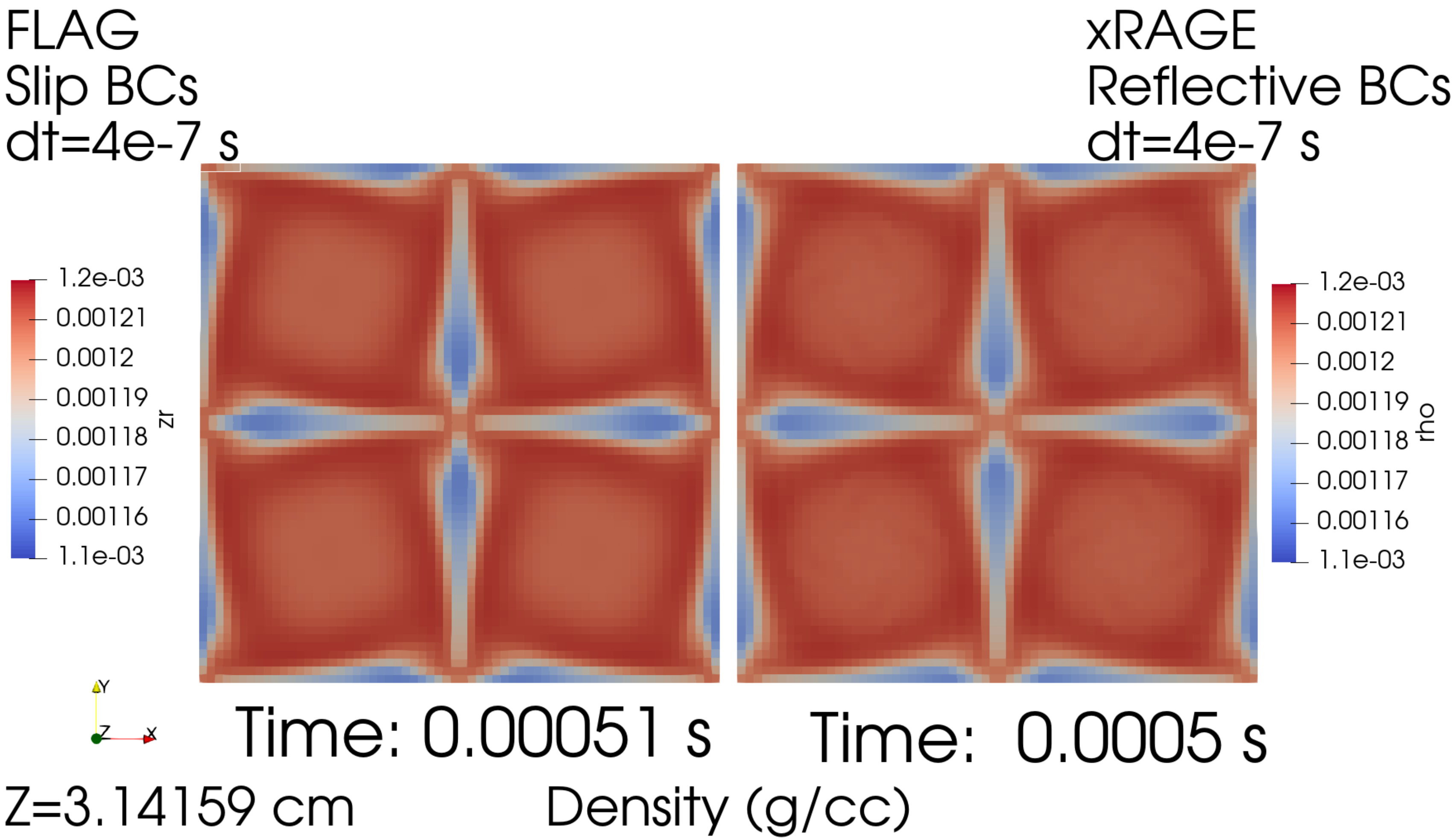
Kinetic Energy, Z center plane

- Qualitative comparisons are consistent between codes up to ~1 ms, after which differences are drastic (much more than individual velocity component comparisons)

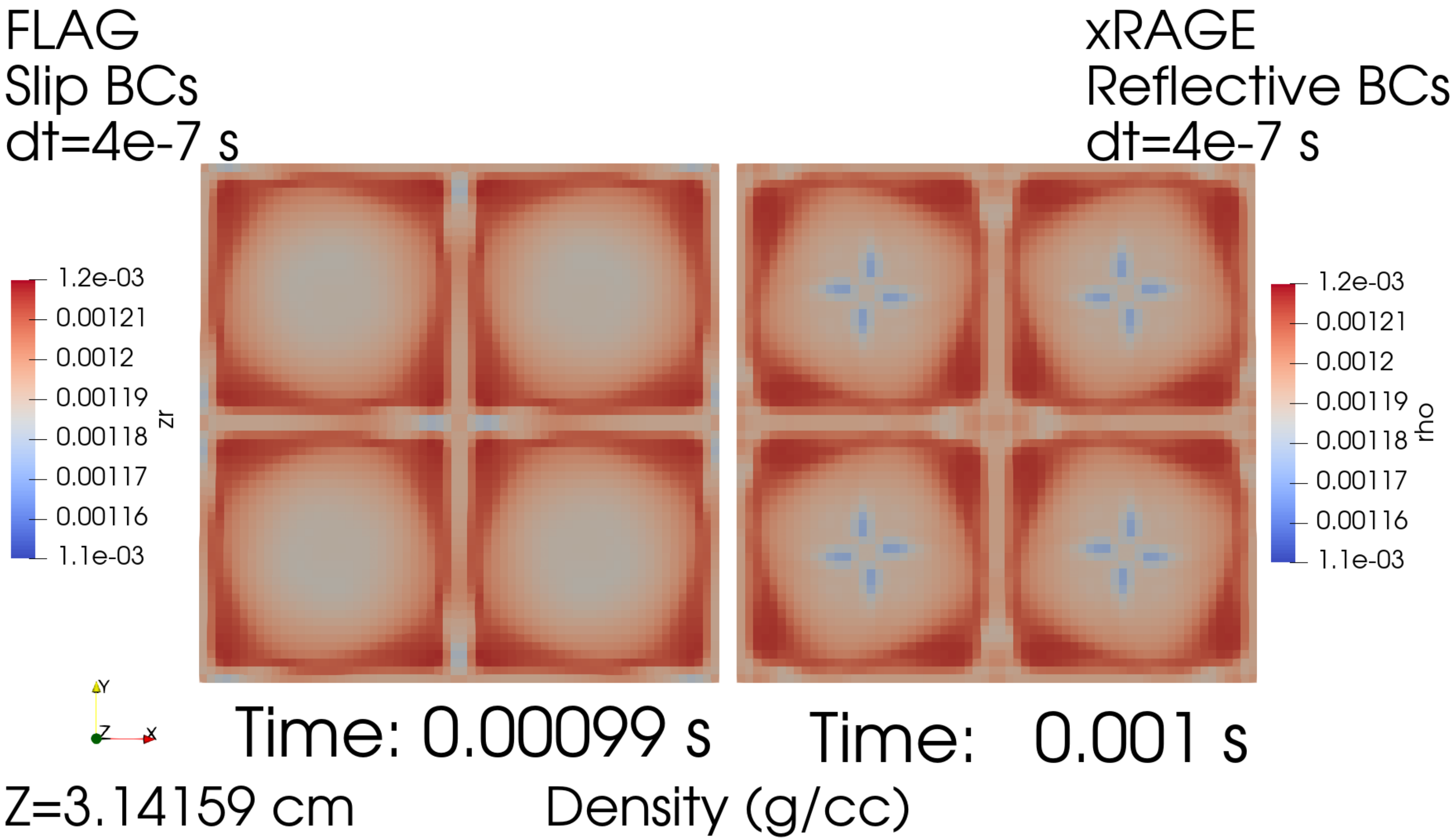
Density, Z center plane



Density, Z center plane



Density, Z center plane

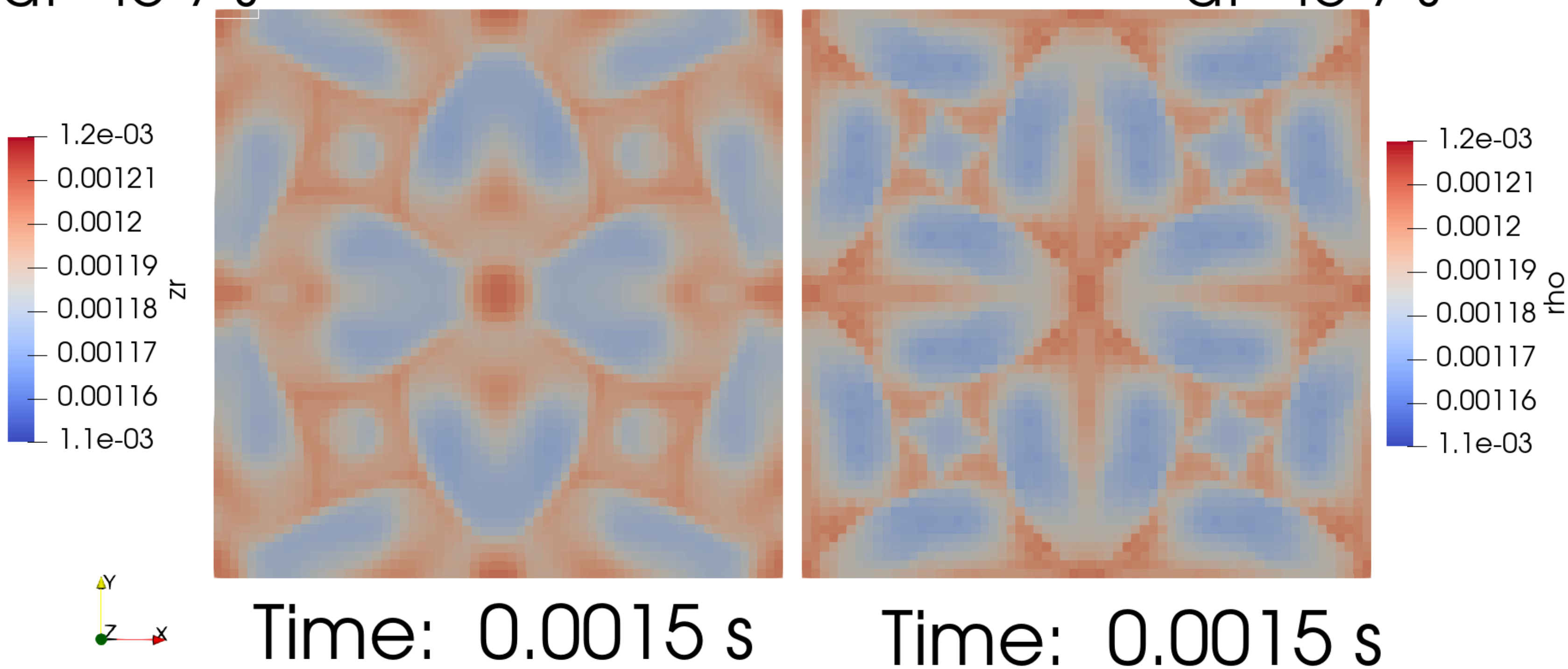


Lower density at the center of vortexes in xRAGE results

Density, Z center plane

FLAG
Slip BCs
dt=4e-7 s

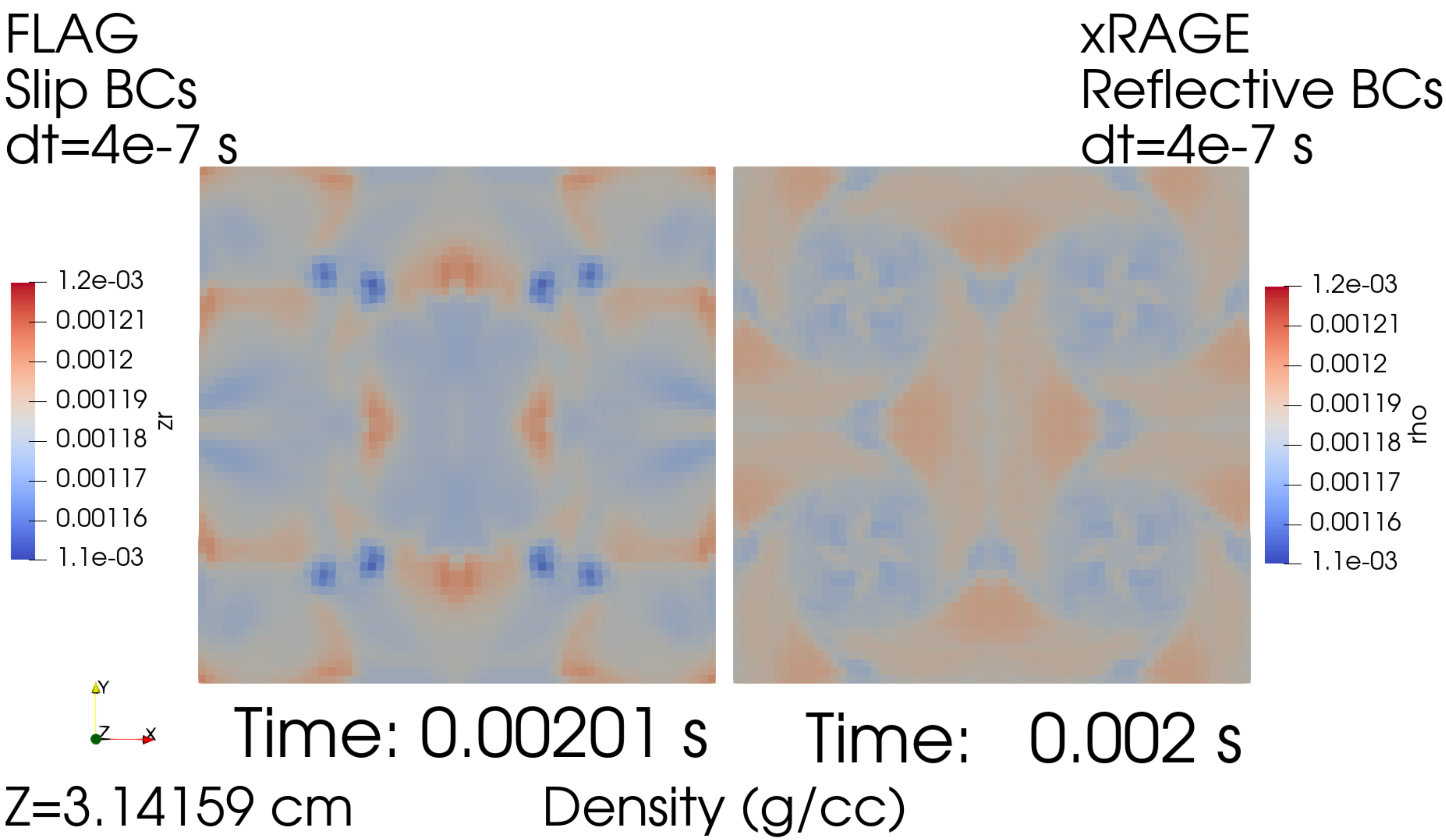
xRAGE
Reflective BCs
dt=4e-7 s



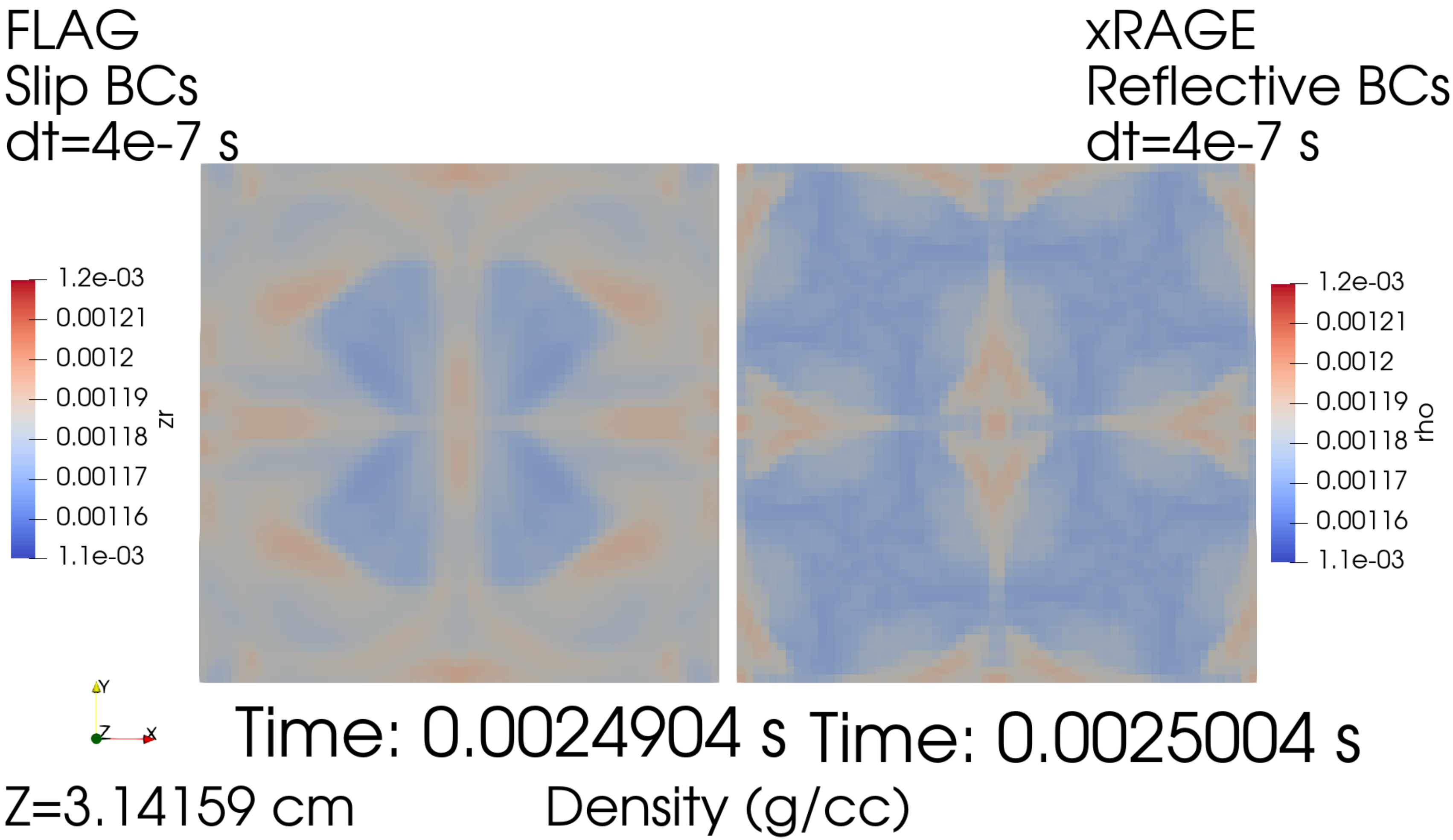
Z=3.14159 cm

Density (g/cc)

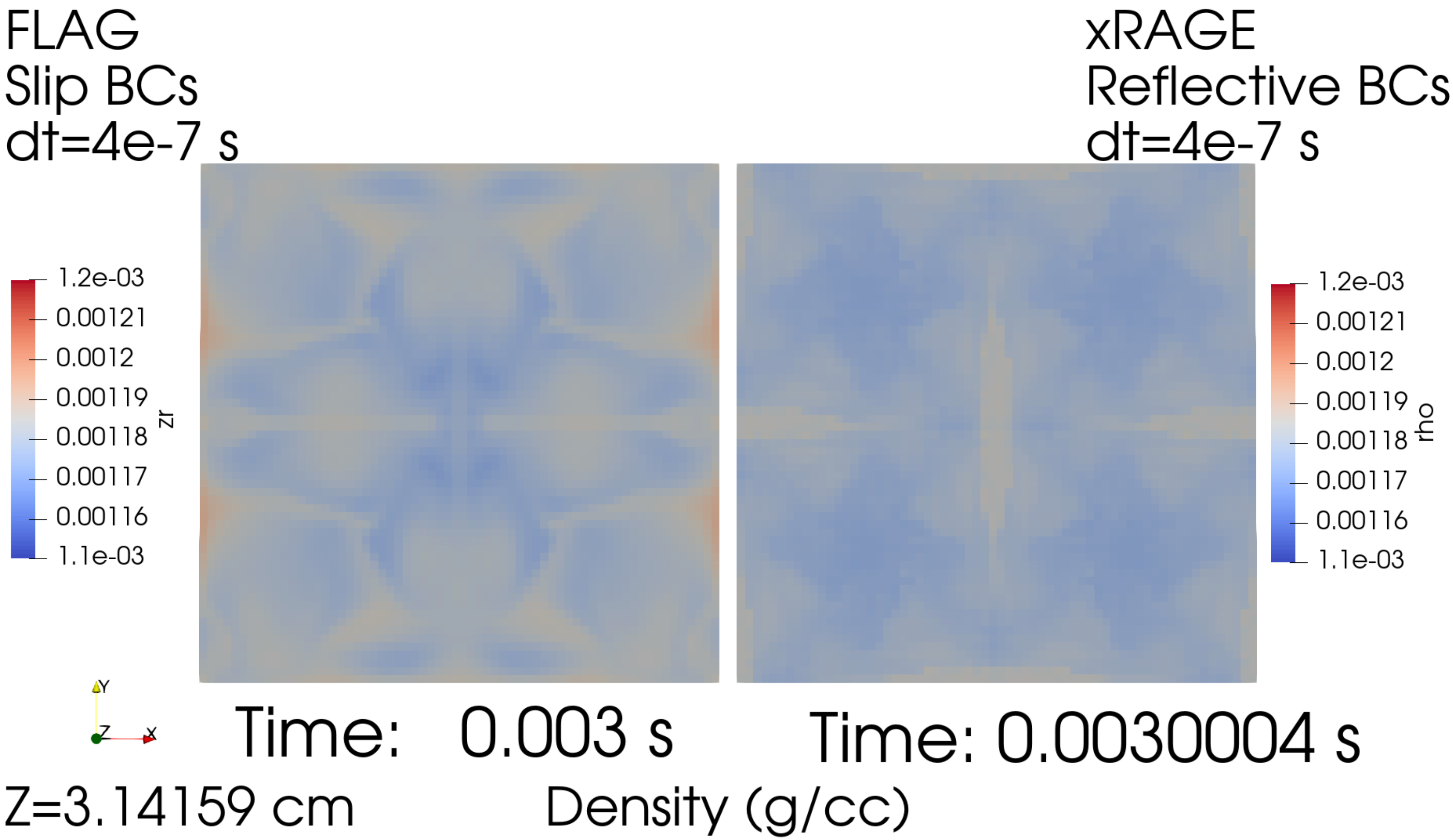
Density, Z center plane



Density, Z center plane



Density, Z center plane



Density, Z center plane

- Differences are noticeable at ~ 1ms and become more distinct at later times

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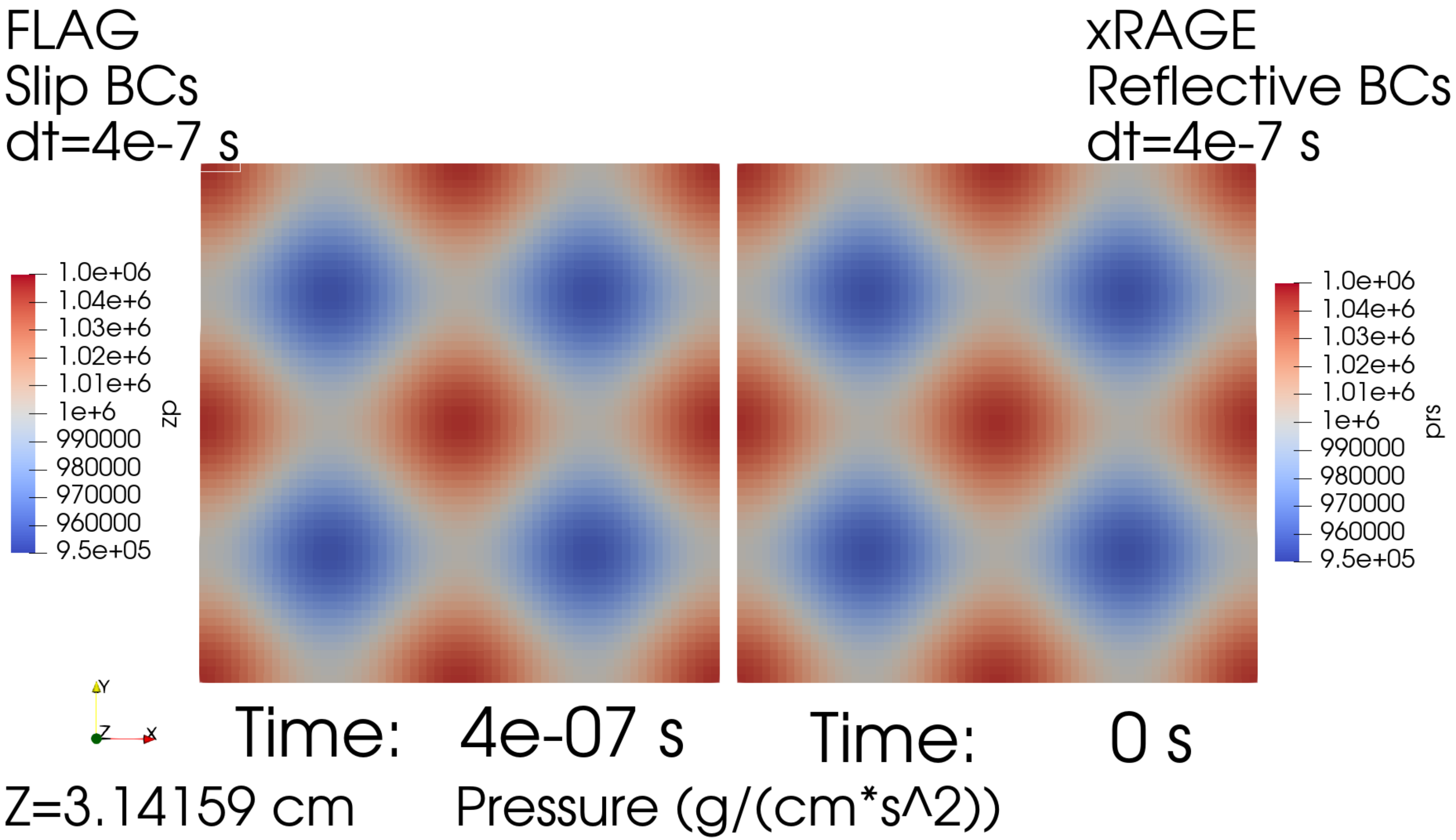
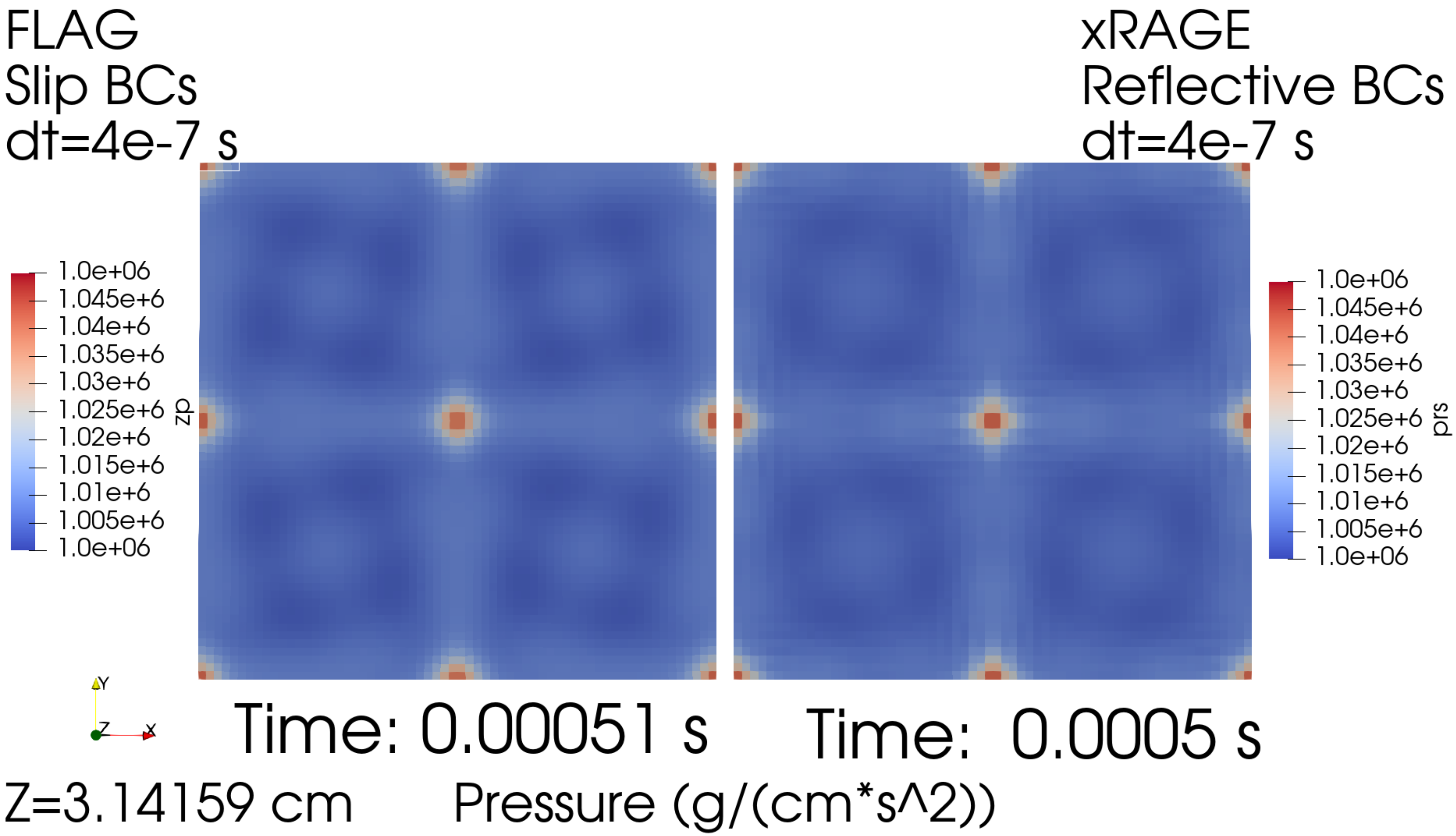
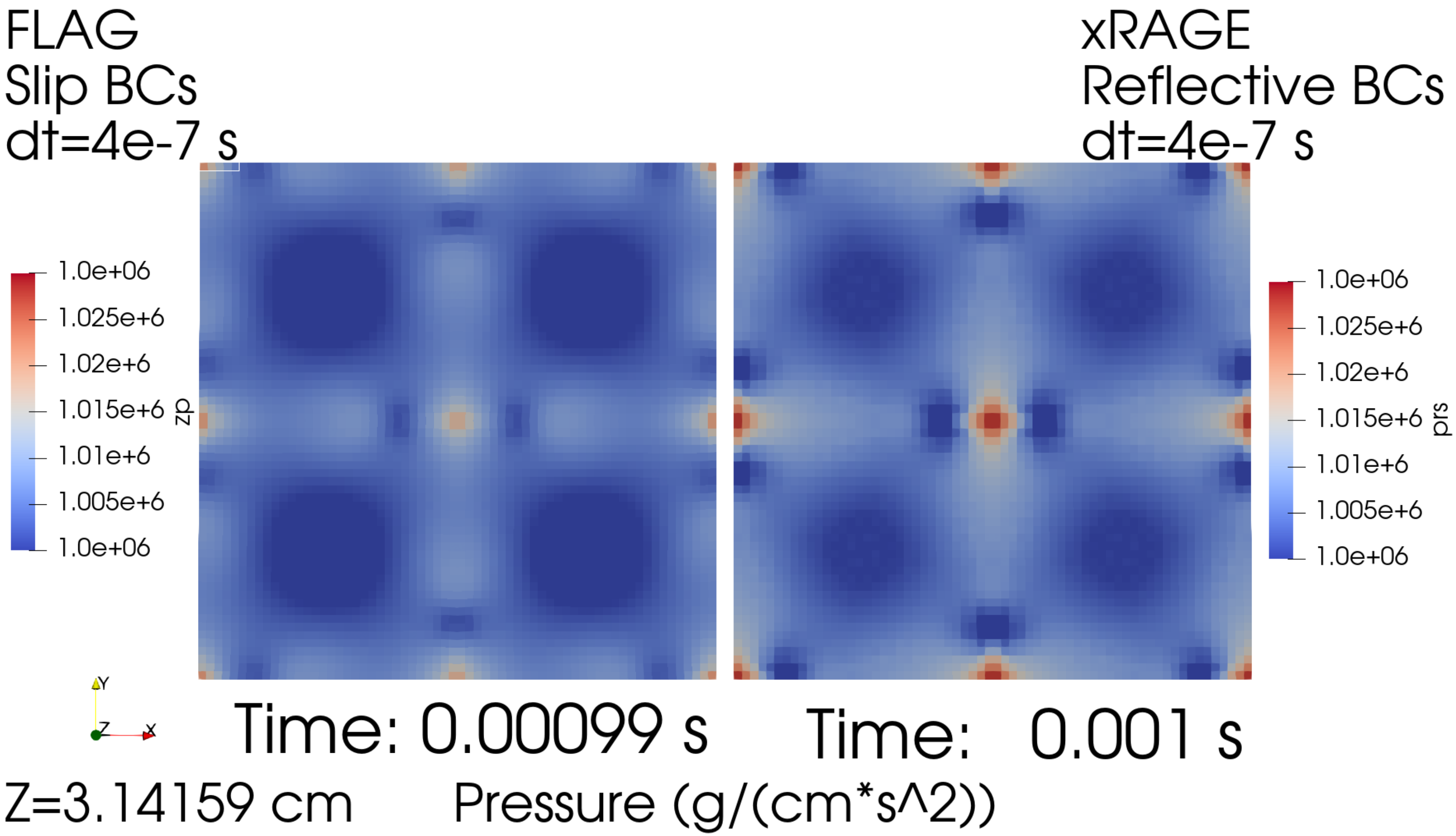
Pressure, Z center plane



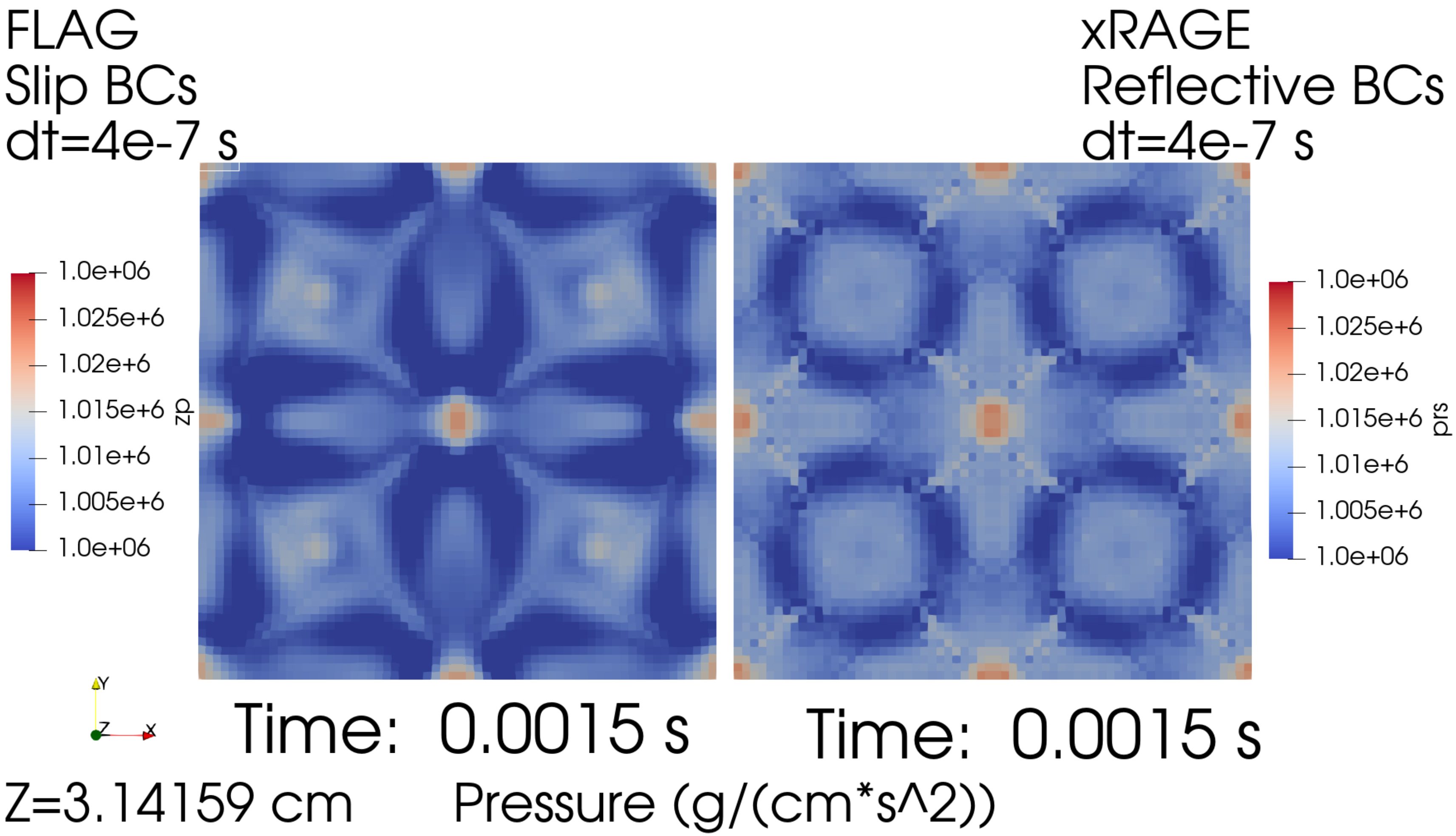
Pressure, Z center plane



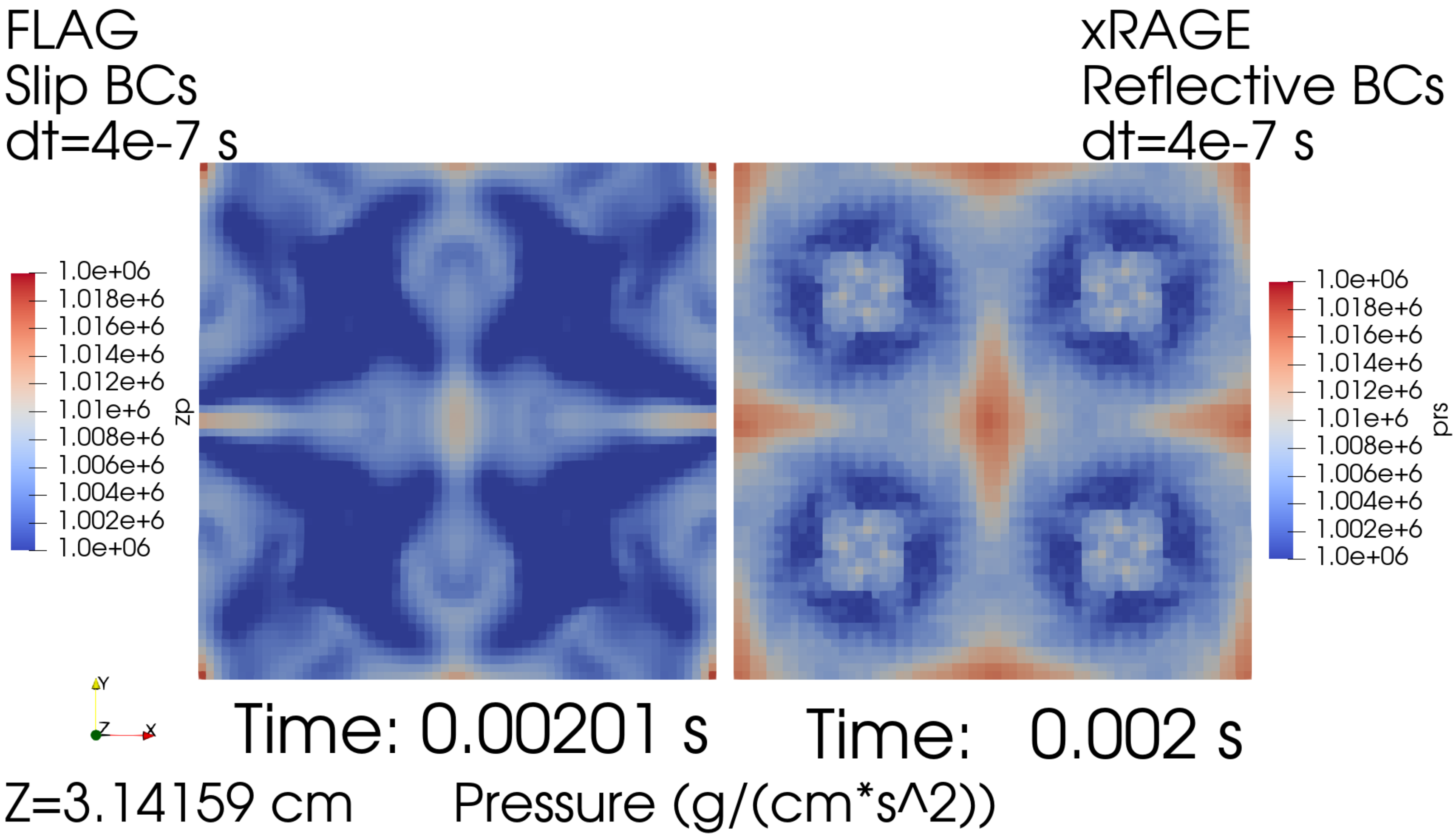
Pressure, Z center plane



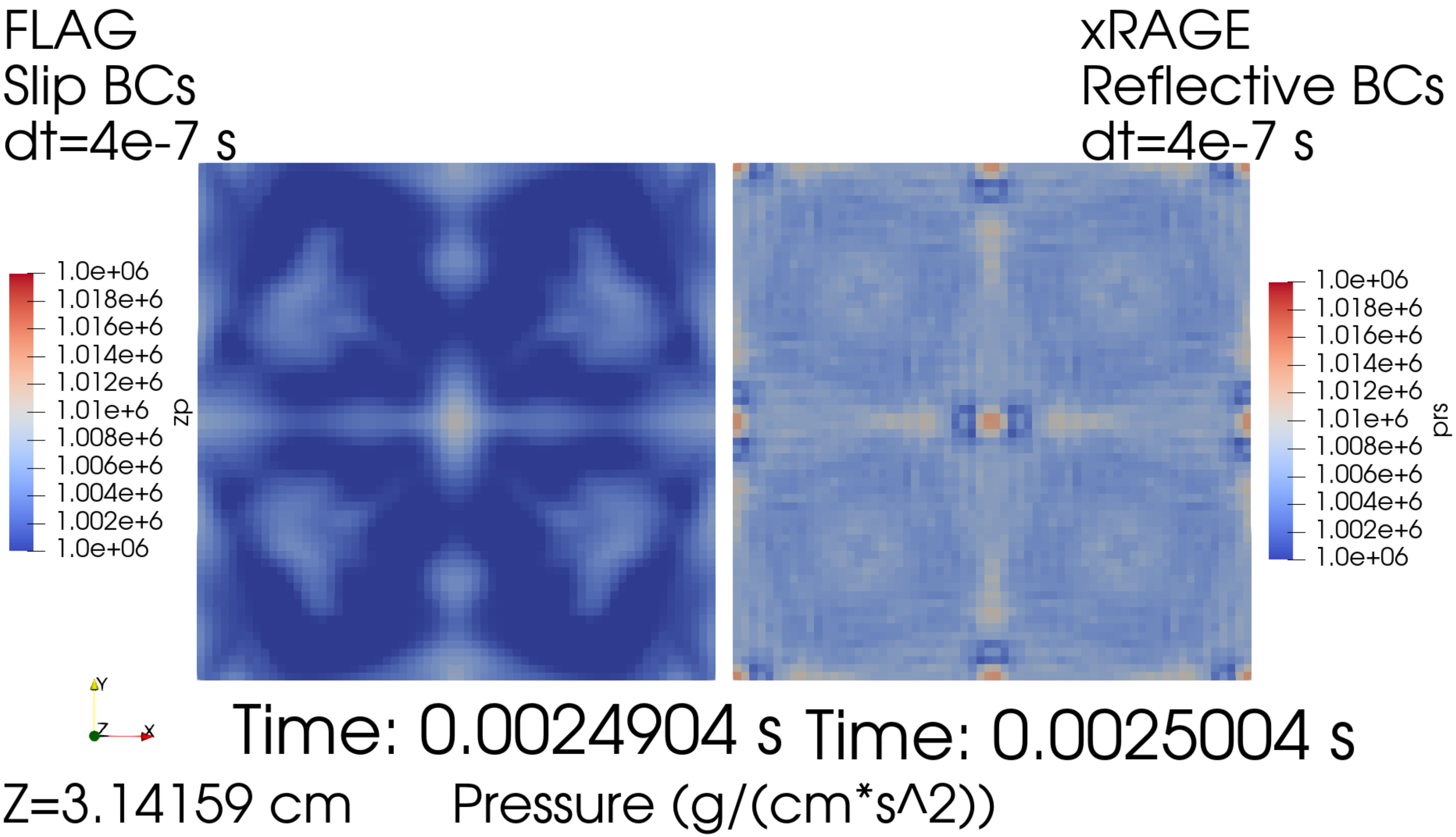
Pressure, Z center plane



Pressure, Z center plane



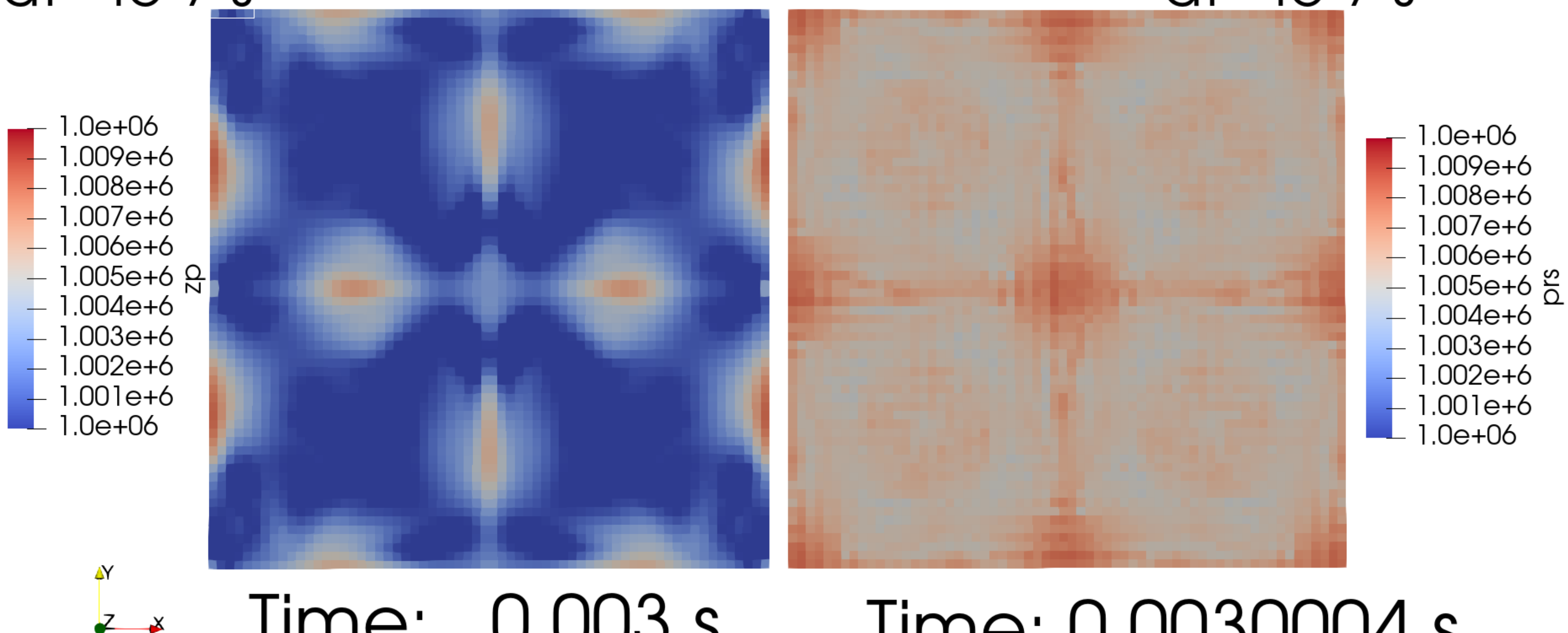
Pressure, Z center plane



Pressure, Z center plane

FLAG
Slip BCs
dt=4e-7 s

xRAGE
Reflective BCs
dt=4e-7 s



Time: 0.003 s

Time: 0.0030004 s

Z=3.14159 cm

Pressure (g/(cm*s^2))

ILES Conclusions

- Initial conditions and problem setup are consistent between codes (good sanity check)
- Differences in BCs are negligible
- All quantities compared show good agreement up to ~1 ms; as the flow transitions to turbulent, differences become significant
- Due to different effective Reynolds numbers (set by the numerics), we can't expect good agreement of instantaneous quantities at late times of a turbulent flow
- Volume-averaged quantities will be used to compare DynamicBHR3 results

DynamicBHR3 Summary

- The contribution function, f, dynamically blends between ILES ($f = 0$) and BHR3 ($f = 1$)

$$f = \gamma \left[1 - \frac{T_{ij}T_{ij}}{T_{ij}R_{ij}} \right]; \; \gamma = \left(\frac{\Delta}{L} \right)^{l}$$

Δ: dx

L: π $(vortex\ size\ for\ TGV\ problem)$

$l = 2\ (for\ 2nd\ order\ numerics)$

R_{ij}: $BHR3\ Reynolds\ Stress$

Resolved Stresses computed with a Helmholz differential filter

$$T_{ij} = \frac{\langle \overline{\rho}\overline{u}_i\overline{u}_j \rangle}{\langle \overline{\rho} \rangle} - \frac{\langle \overline{\rho}\overline{u}_i \rangle}{\langle \overline{\rho} \rangle} \frac{\langle \overline{\rho}\overline{u}_j \rangle}{\langle \overline{\rho} \rangle}$$

$\langle \cdot \rangle$: $Helmholtz\ filtered\ quantity$

- The contribution function is computed each time step and scales the BHR3 contributions to conservation of mass, momentum, and energy
- Additional details on the derivation are given by Grinstein et al. [1]

[1] Grinstein, F. F., J. A. Saenz, R. M. Rauenzahn, Massimo Germano, and D. M. Israel. "Dynamic bridging modeling for coarse grained simulations of shock driven turbulent mixing." *Computers & Fluids* 199 (2020): 104430.

Volume-Averaged Quantities

- Resolved Kinetic Energy: $$KE = \frac{1}{V}\sum_z 0.5(\bar{u}^2 + \bar{v}^2 + \bar{w}^2)dz$$

$\bar{\cdot}$: *implicit grid filtered or resolved quantity*

V : *domain volume*

z : *zone*

dz : *zone volume*

u, v, w : *velocity components*

- Modeled Kinetic Energy: $$TKE = \frac{1}{V}\sum_z 0.5\left(\frac{R_{11} + R_{22} + R_{33}}{\rho}\right)dz$$

R_{ij}: *Reynolds Stress Tensor*

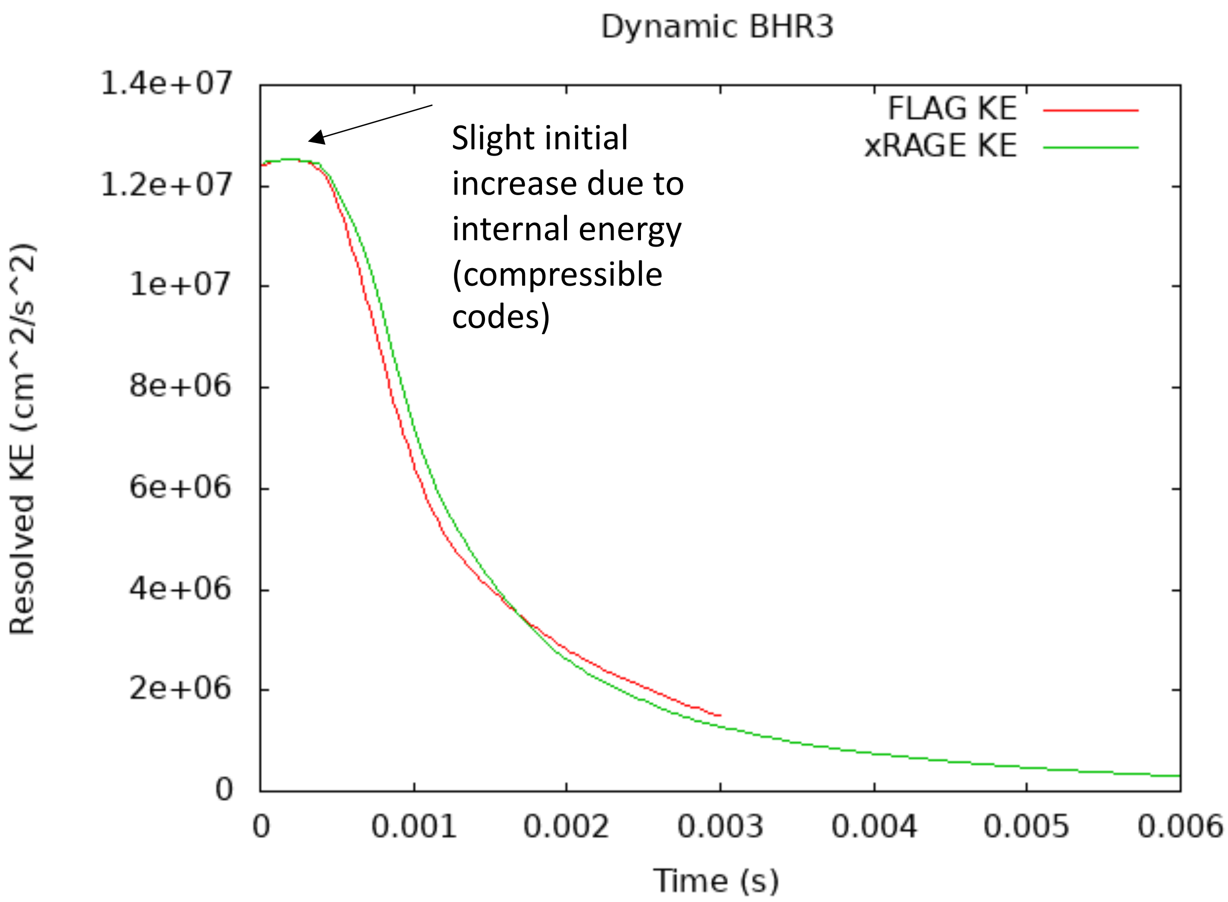
ρ : *density*

- Total Kinetic Energy = KE + TKE

Units (cm^2/s^2)

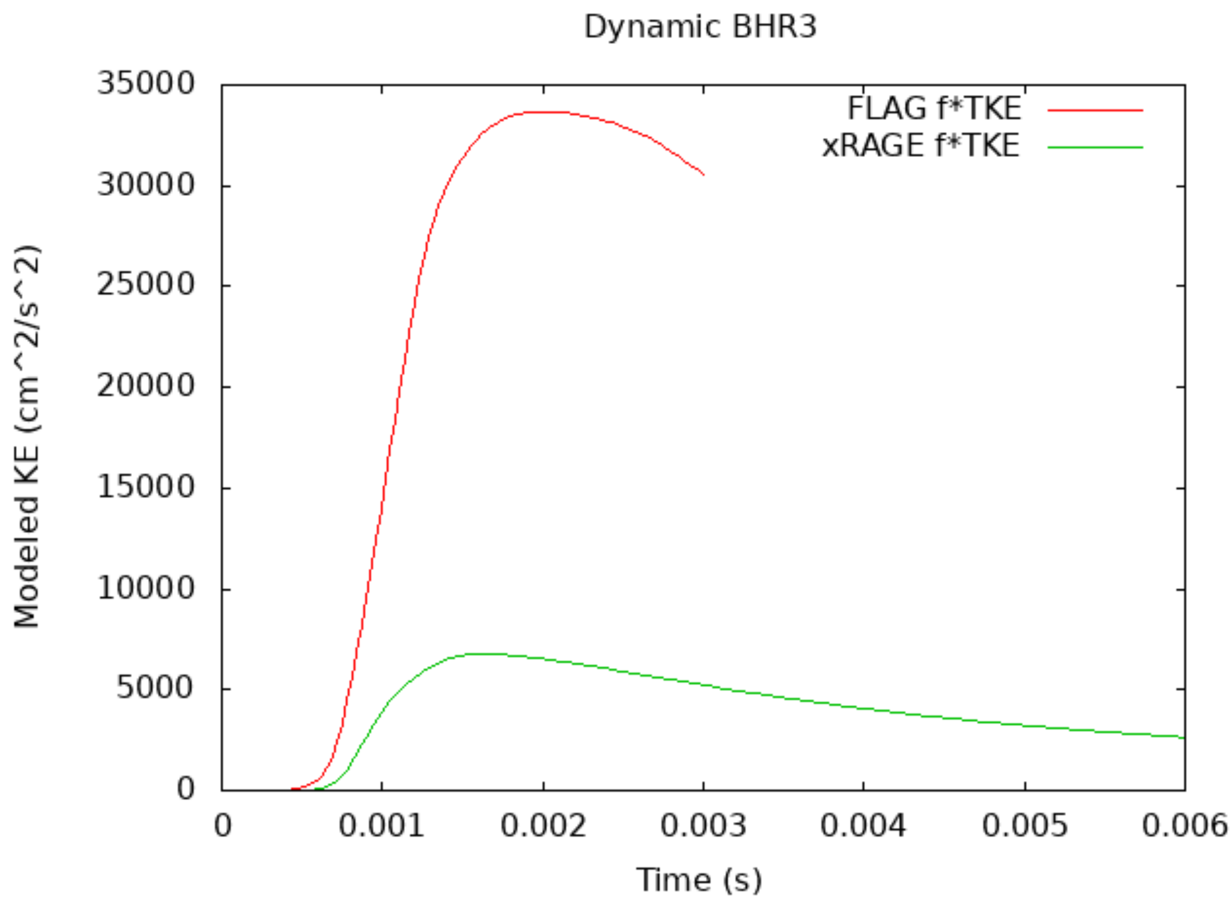
DynamicBHR3 FLAG/xRAGE Comparisons

- Resolved Kinetic Energy
- Reasonable comparison between codes



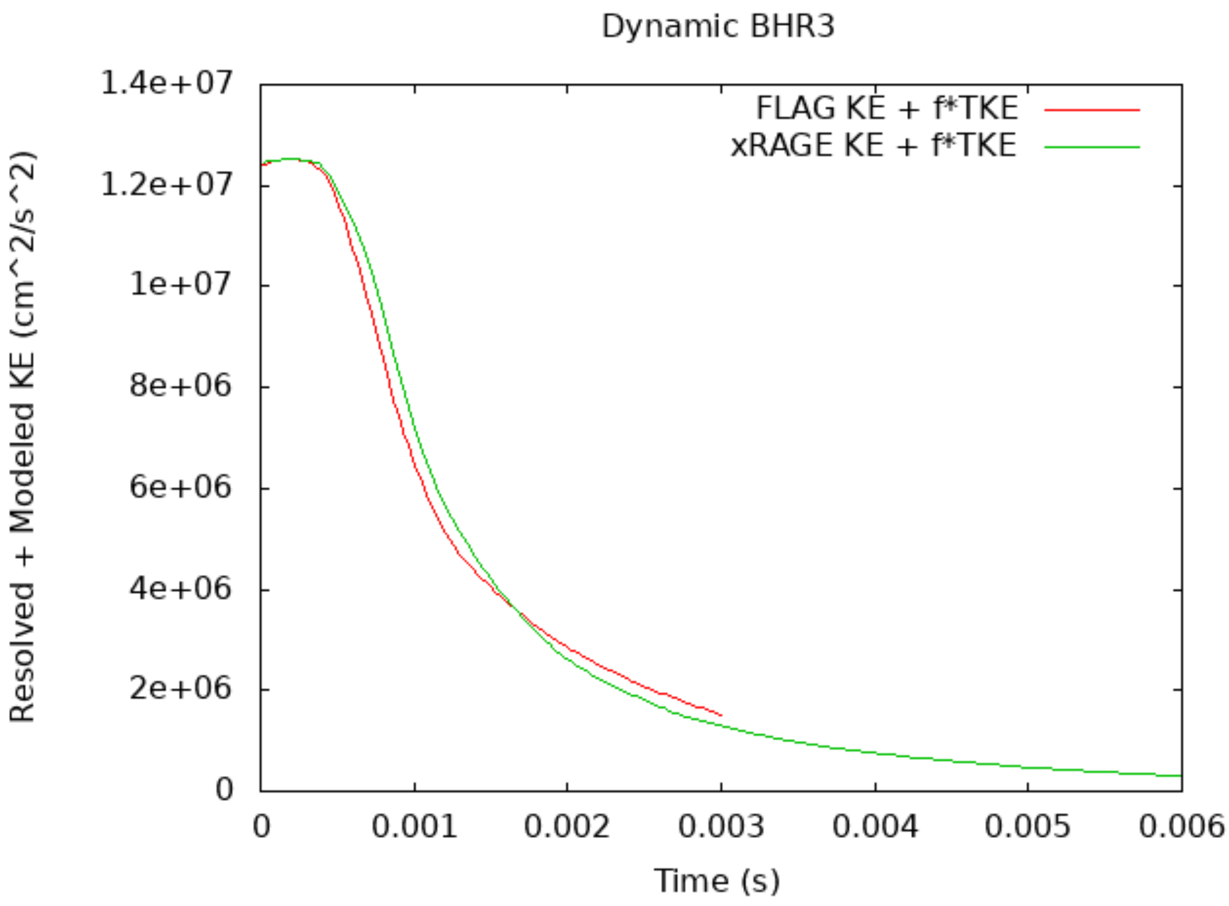
DynamicBHR3 FLAG/xRAGE Comparisons

- Modeled Kinetic Energy; contribution function times TKE
- Factor ~5 difference between codes
- TKE evolution in BHR3 when running DynamicBHR3 is very different between FLAG/xRAGE (more on that in two slides)



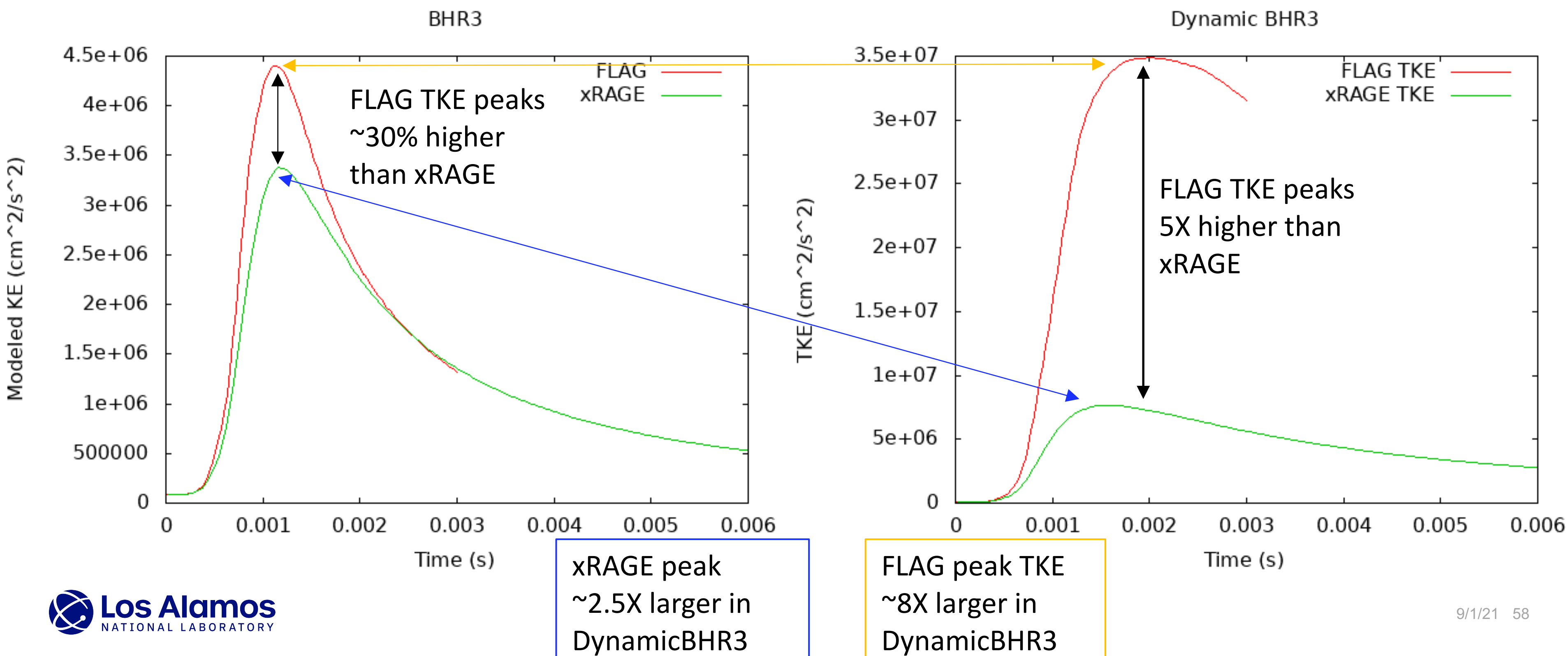
DynamicBHR3 FLAG/xRAGE Comparisons

- Total (resolved + modeled) Kinetic Energy
- Modeled contribution is several orders of magnitude smaller than the resolved contribution, so this looks similar to the resolved KE comparison



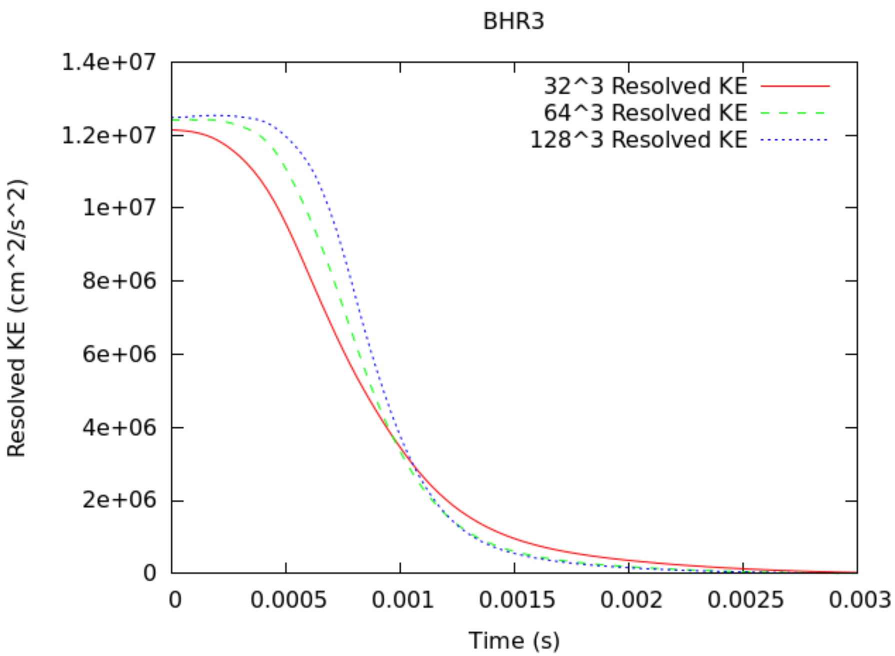
FLAG/xRAGE Comparisons

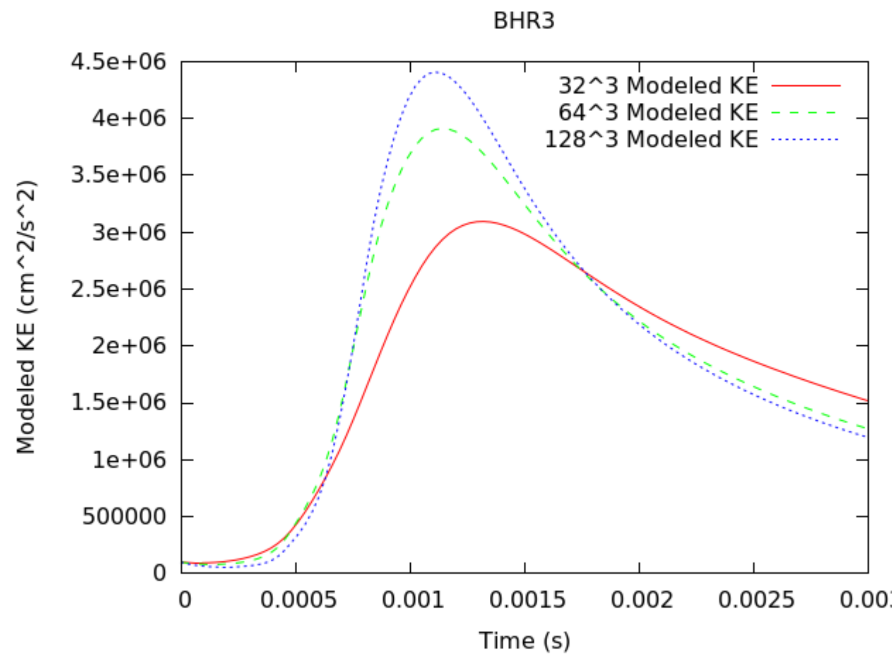
- Two separate runs with each code: one using BHR3, and one using DynamicBHR3
- Comparing the evolution of TKE in each case
- Initial KE is ~1.2e7; how can FLAG's TKE evolve to ~3.5e7?
- FLAG TKE peak is higher in BHR3 and significantly higher in DynamicBHR3 compared to xRAGE (y-scale is different in figures)



FLAG Resolution Study: BHR3

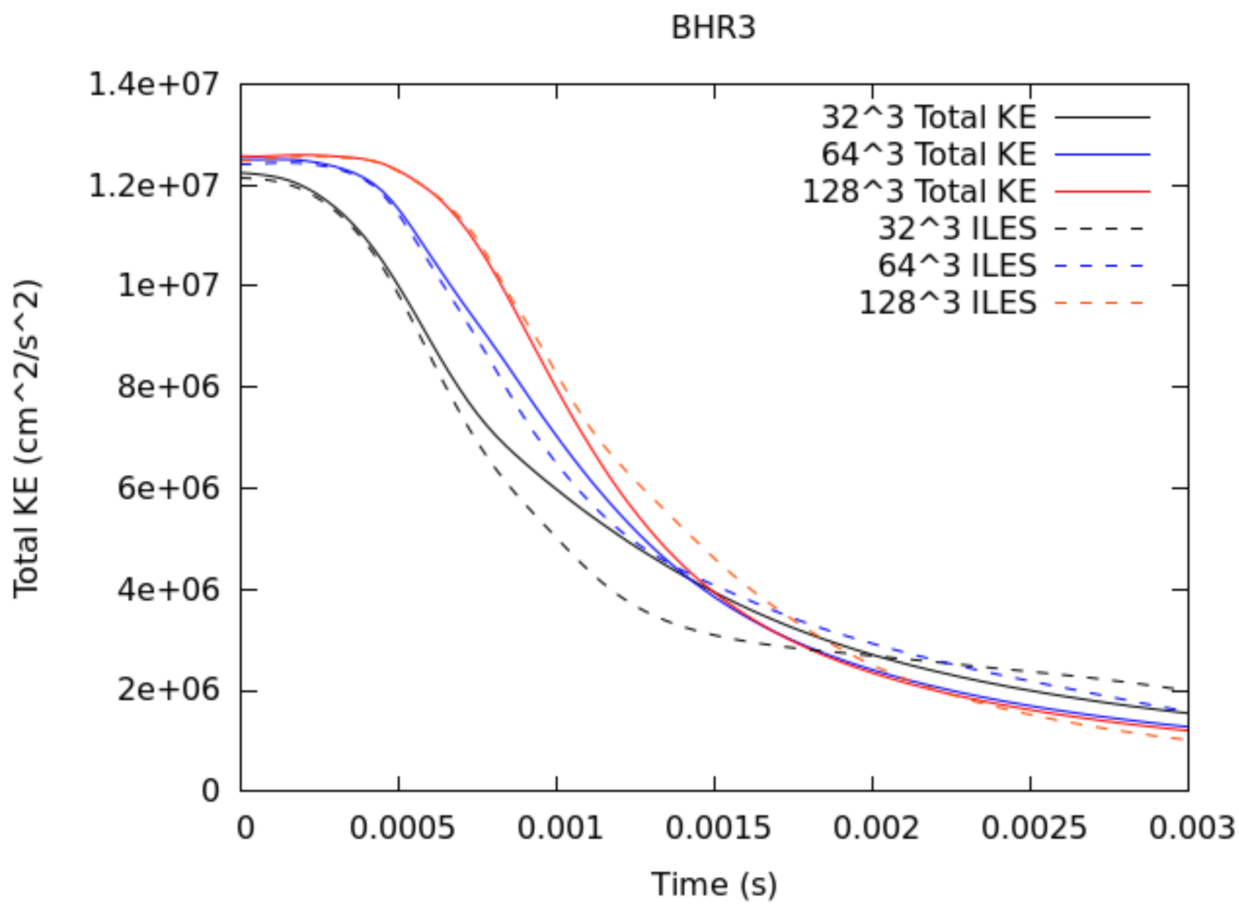
- Resolved and modeled KE increase with resolution until late times; more resolved scales yields higher peak TKE
- Solution is not mesh-independent for this problem at these three resolutions
- This is a transition from laminar to turbulent problem; inherently difficult for turbulence models, which assume initial turbulent flow. **This is a code verification exercise – I'm not advocating that BHR3 is appropriate for a transition problem like this.**





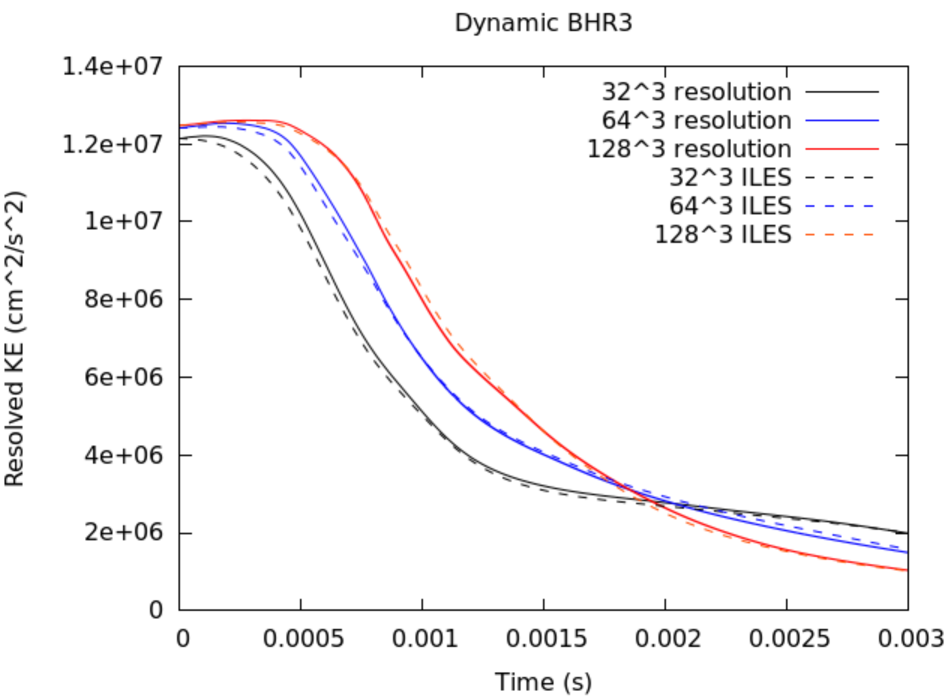
FLAG Resolution Study: BHR3

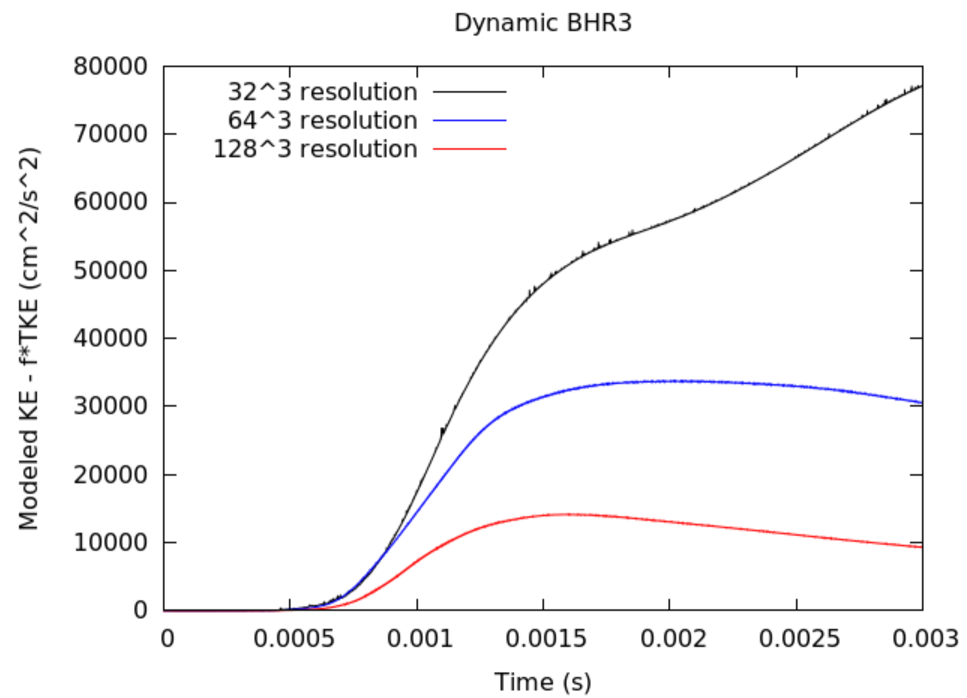
- Total (resolved + modeled) Kinetic Energy from BHR3 runs
- ILES resolved KE are shown as well
- Total KE from BHR3 does not converge to the resolved ILES KE (128^3 is not really better than 64^3)



FLAG Resolution Study: DynamicBHR3

- Resolved and modeled KE (f*TKE) are shown below
- Trends are as expected:
  - More KE is resolved with additional resolution
  - Less KE is modeled with additional resolution
- Note that modeled KE is several orders-of-magnitude lower than resolved KE, so resolved KE is similar to ILES resolved KE



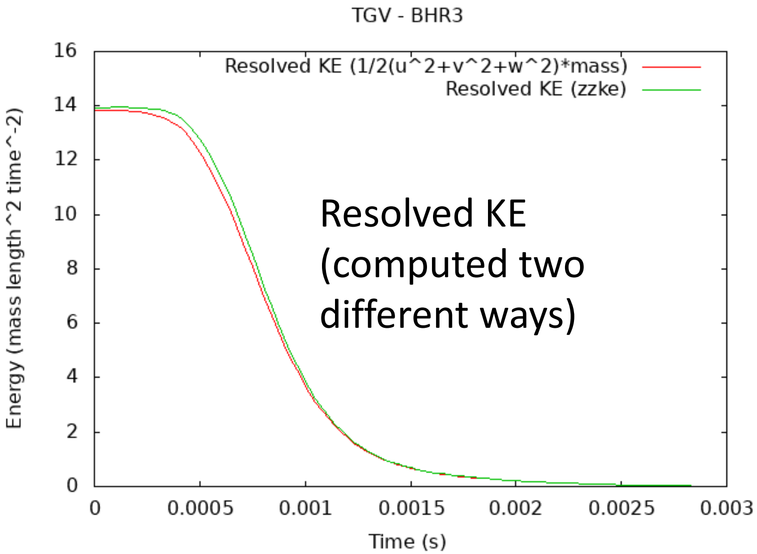


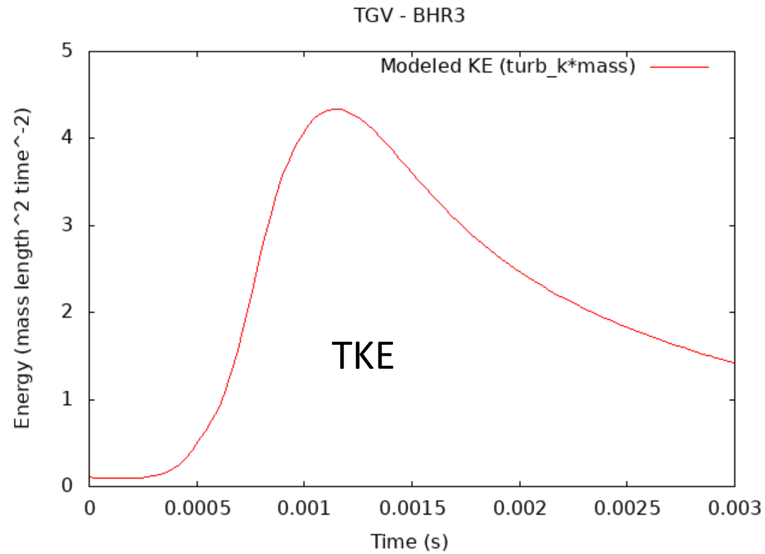
Energy Conservation – FLAG

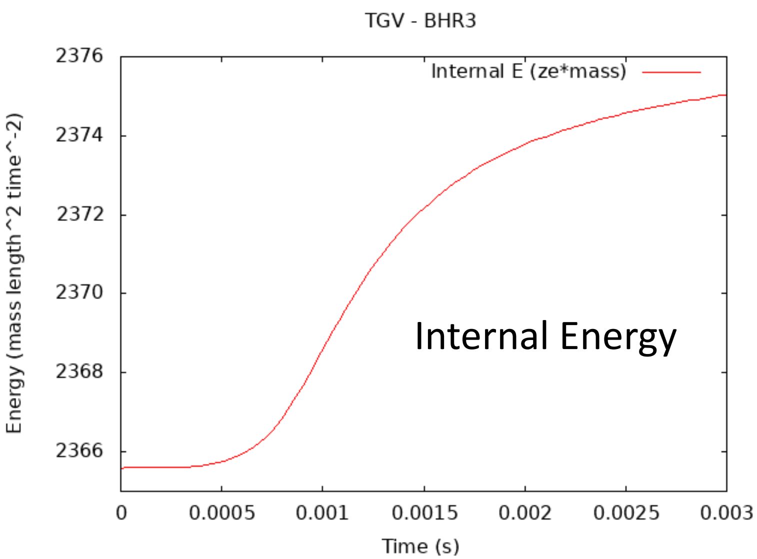
- Evolution of TKE in FLAG increases significantly more in FLAG than it does in xRAGE when running DynamicBHR3
- BHR3 equations are unaltered in DynamicBHR3, but given that it operates anywhere between ILES (more turbulent fluctuations resolved) and BHR3 (more dissipative and dampened fluctuations), some differences are expected between BHR3 and DynamicBHR3
- We want to check the conservation of total energy during a calculation: total energy = internal energy + resolved kinetic energy + modeled kinetic energy
- It is NOT possible to discretely conserve all quantities exactly (mass, momentum, internal energy, kinetic energy, etc.)
- FLAG conserves internal energy in a 'compatible' way to also conserve total energy only when running pure Lagrangian [2]; ALE introduces additional error
- Note that xRAGE conserves total energy; fundamental difference between codes

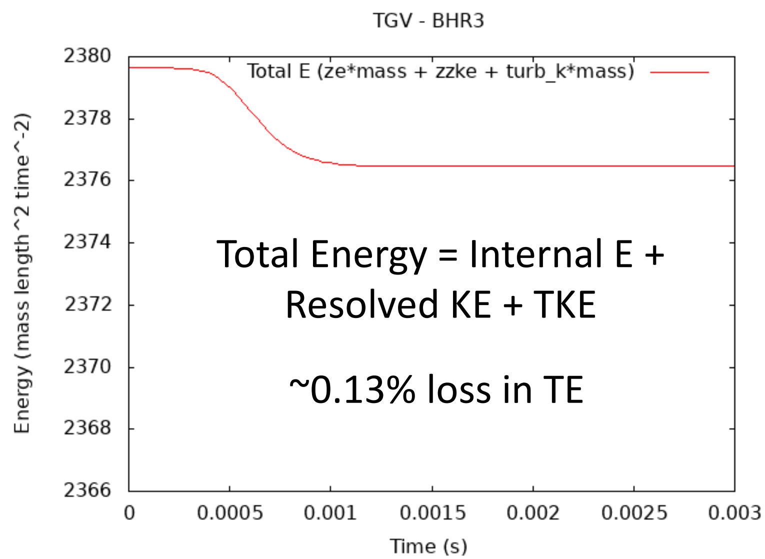
[2] E. J. Caramana et al.,"Construction of Compatible Hydrodynamics Algorithms Utilizing Conservation of Total Energy," JCP 146: 227-262, 1998.

Energy Conservation – FLAG BHR3









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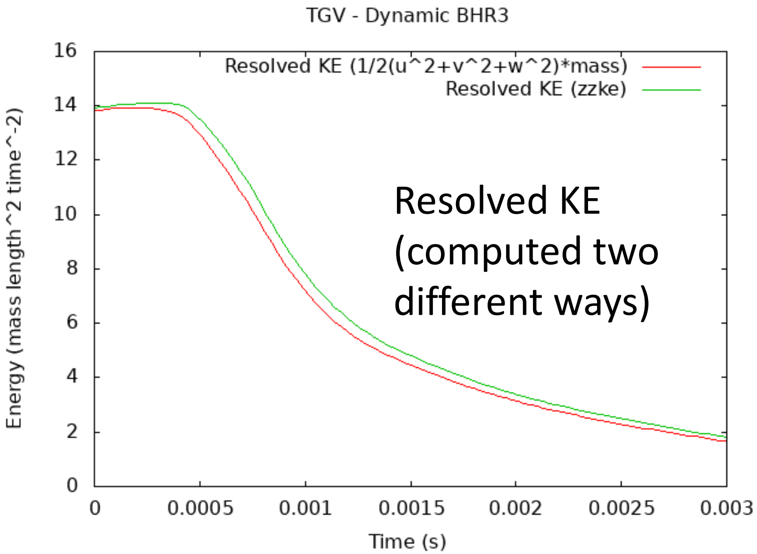
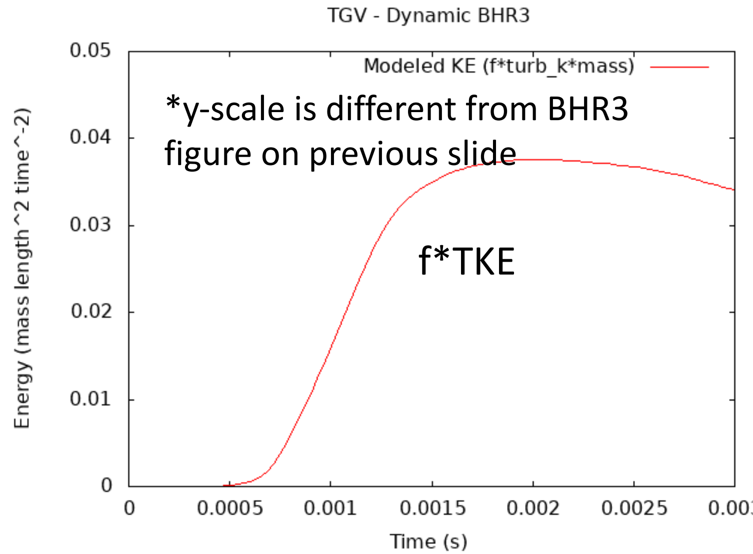
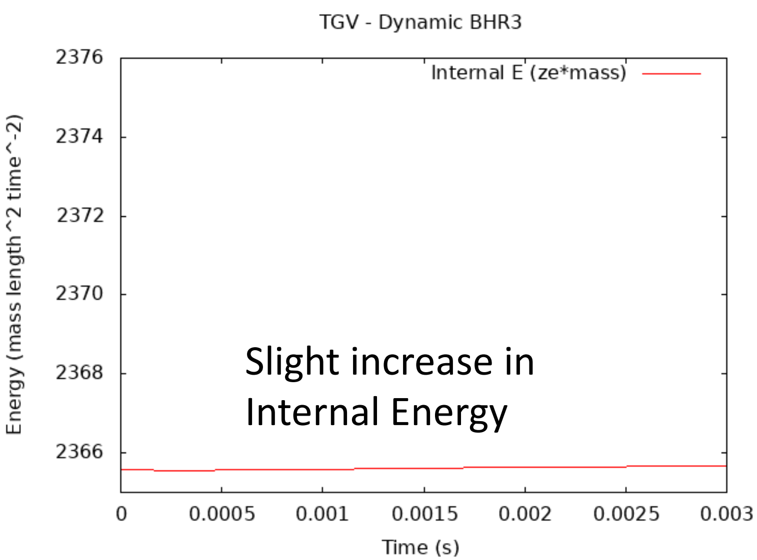
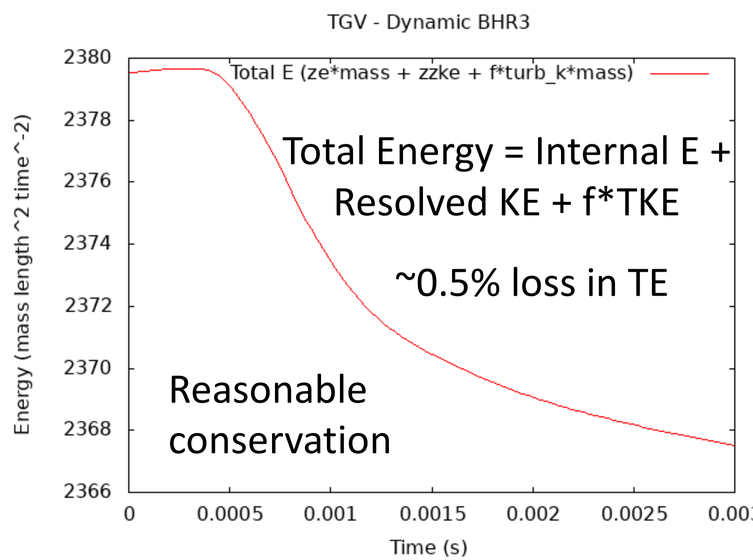
Energy Conservation – FLAG Dynamic BHR3









FLAG DynamicBHR3 Conclusions

- Conservation of total energy is reasonable
- Modeled contributions show the expected trends under mesh refinement, but the magnitudes are very different from xRAGE
- Difficult to determine where these differences come from
  - DynamicBHR3 implementation?
  - BHR3 implementation? Baseline BHR3 comparison is ~30% different between codes
  - Fundamental difference in codes (conservation of total energy vs internal energy, numerics)?
  - Difference in setup (e.g. clipping strategy in BHR3 source/sink terms)?

Future Work

- Investigate FLAG's kinetic energy fixup option (iadvkefixup option under the advection node)
  - This subtracts the increase in kinetic energy from internal energy such that total energy is conserved (similar behavior as xRAGE)
- Use a physical viscosity (Navier-Stokes calculations) that is larger than the numerical diffusion error
  - This will set the Reynolds number of the flow to be exactly the same for both codes and should lead to better agreement at late times
- Perform similar 1D and 2D code-to-code verification of BHR3 as was previously done with BHR2 by Denissen et al. [1]
  - BHR3 has not yet been as rigorously tested between the two codes

[1] N. Denissen, J. Fung, J. Reisner, and M. Andrews. "Implementation and Validation of the BHR Turbulence Model in the FLAG Hydrocode." LA-UR-12-24386, 2012.